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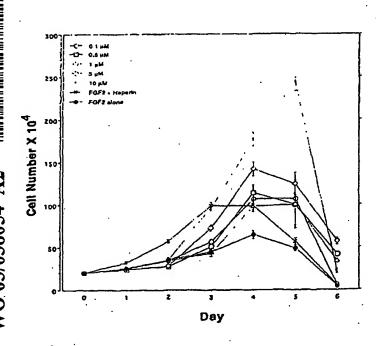
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(54) Title: STRUCTURE-BASED DESIGN AND SYNTHESIS OF FGF INHIBITORS AND FGF MODULATOR COMPOUNDS



(57) Abstract: The present invention provides methods and compositions for modulating FGF-signaling and activities associated therewith, such as mitogenesis and angiogenesis. In particular, the crystal structure provides invention coordinates for a ternary complex of an FGF-receptor, and FGF ligand, and a third compound, sucrose octasulfate, that binds to the FGF receptor and ligand to promote formation and dimerization of the ternary complex. Screening methods are provided by which novel agonists and antagonist for FGF-mediating signaling and activities may be identified using these crystal structure coordinates. Exemplary compounds are also provided that have novel utilities as agonists or antagonists of FGP-mediated signaling and activites.

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STRUCTURE-BASED DESIGN AND SYNTHESIS OF FGF INHIBITORS AND FGF MODULATOR COMPOUNDS

CROSS-REFERENCE TO RELATED APPLICATION(S)

Priority is claimed under 35 U.S.C. § 119(e) to U.S. provisional patent

application serial no. 60/335,583 filed on October 31, 2001, which is incorporated herein by reference in its entirety.

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STATEMENT REGARDING FEDERALLY SPONSORED RESEARCH AND/OR DEVELOPMENT

This invention was made with Government support under Grant Nos. 1R01-DE13686-01, 1RO1-HL52622 and 1RO1-HL62244, awarded by the National Institutes of Health. The United States Government may have certain rights to this invention pursuant to the terms of those grants.

FIELD OF THE INVENTION

The present invention relates to a class of proteins known as fibroblast growth factor (FGF) proteins or FGF ligands. The invention also relates to receptors, known as fibroblast growth factor receptors (FGFRs), that recognize and specifically bind to FGF proteins. More specifically, the invention relates to novel uses of compounds such as sucrose octasulfate (SOS), myo-inositol hexasulfate, cyclodextrin (particularly sulfated β -cyclodextrin) and suramin to modulate biological activity associated with FGF. The invention also relates to uses of such compounds to modulate dimerization of FGF - FGFR complexes.

BACKGROUND OF THE INVENTION

The mammalian fibroblast growth factor (FGF) family comprises at least 22 related polypeptides that are generally known in the art as FGF1 - FGF22. These polypeptides are known to be essential for normal human development and, moreover, are

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involved in the pathologies of many human diseases such as cancer and dwarfism, to name a few. For reviews, see McKeehan et al., Progress in Nucleic Acid Research and Molecular Biology 1998, 59:135-176; Nishimura et al., Biochim. Biophys. Acta. 2000, 1492:203-206; and Yamashita et al., Biochem. Biophys. Res. Commun. 2000, 277:494-498.

The diverse effects of FGF polypeptides are mediated by at least four receptor tyrosine kinase polypeptides, referred to collectively as the FGF receptors (FGFRs), and known individually as FGFR1 - FGFR4. These FGFR polypeptides comprise an extracellular domain, a single transmembrane helix domain, and a cytoplasmic portion with tyrosine kinase activity. The FGFR polypeptides' extracellular domain itself has at least three immunoglobulin (Ig)-like domains, which are referred to respectively as D1 - D3. The receptors' binding specificity resides in, and is therefore incurred by, the D2 and D3 and by the short linker polypeptide sequence between those two domains. See, Plotnikov et al., Cell 1999, 98:641-650; Plotnikov et al., Cell 2000, 101:413-424; and Stauber et al., Proc. Natl. Acad. Sci. U.S.A. 2000, 97:49-54 for a more detailed discussion.

FGF-induced FGFR dimerization is a key event in FGF signaling processes (Schlessinger, 2000). However, whereas other known growth factors such as platelet-derived growth factor (PDGF), neurotrophic growth factor (NGF) and colony stimulating growth factor 1 (CSF1) are themselves dimeric molecules, the FGF polypeptides are monomeric molecules and do not form dimers by themselves in solution. Consequently, FGF polypeptides cannot induce receptor dimerization by themselves and instead require soluble or cell surface-bound heparan sulfate proteoglycans (HSPG) to promote FGFR dimerization and subsequent activation.

The crystal structure determined for one FGF-FGFR-heparin complex (see, Schlessinger et al., Molecular Cell 2000, 6:743-750) indicates one putative mechanism by which heparin may facilitate FGFR dimerization. Without being limited to any particular theory or mechanism of interaction, such dimerization is believed to occur according to a "two end" model in which the non-reducing end of heparin interacts with heparin binding sites of the FGF and FGFR polypeptides to promote formation of a ternary FGF:FGFR:heparin complex of 1:1:1 stoichiometry. A second ternary FGF:FGFR:heparin complex is then recruited to this first complex by means of interactions of (i) FGFR, FGF and heparin in the first complex, with (ii) FGFR in the second complex.

The central role played by heparin for the dimerization, and hence activation, of FGF receptor polypeptides makes heparin's interactions with FGF and FGFR attractive targets for compounds which may modulate FGF receptor activity. Compounds that modulate this interactions would be useful as therapeutic agents, e.g., for the treatment of disorders associated with FGFR activity. However, the capabilities that are currently available for large-scale preparation of homogenous heparin oligosaccharides suitable for therapeutic applications are severely limited (see, Pervin et al., Glycobiology 1995, 5:83-95). There exists, therefore, a need for identifying other molecules which modulate the dimerization of FGF receptor polypeptides (e.g., by interfering with the stabilizing interactions of heparin), and which may therefore be useful, e.g., as therapeutic agents to modulate FGF receptor activity and to treat disorders associated with such activity.

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It has also been suggested that some other sulfated compounds may also bind to an FGF ligand in place of heparin. For example, sucrose octasulfate (SOS) is marketed as an aluminum salt in CARAFATE® or sucralfate, a pharmaceutical composition used to treat duodenal ulcers (see, the *Physician's Desk Reference*, 54 Ed., 2000, Medical Economics Company, Inc., Montvale, New Jersey). The mechanisms by which the compound heals ulcers are largely unknown. However, it has been suggested that SOS may promote healing by binding to and stabilizing FGFs against denaturation in the acidic pH of the stomach (Folkman *et al.*, Ann. Surg. 1991, 214:414-425; see, also, Volkin *et al.*, Biochimica et Biophysica Acta 1993, 1203:18-26). A crystal structure of SOS bound to FGF1 also shows that SOS stabilizes FGF by neutralizing the positively charged high affinity heparin binding residues in FGF (Zhu *et al.*, Structure 1993, 1:27-34). The FGF ligand is also known to bind inositol hexasulfate (Pineda-Lucena, J. Mol. Biol. 1994, 42:81-98) and to suramin (Middaugh *et al.*, Biochemistry 1992, 31:9016-9024). However, whereas inositol hexasulfate may function as a substitute for heparin to activate FGF signaling (Pineda-Lucena *et al.*, supra), suramin actually inhibits signaling by FGF (Middaugh *et al.*, supra).

Despite these teachings, it is not currently known in the art whether these compounds may also mediate or inhibit dimerization of FGF receptor molecules. Indeed, the exact mechanism(s) by which such compounds activate or inhibit FGF signaling remain unknown. The knowledge of such particular interactions may greatly facilitate the identification and/or screening of novel compounds that may be used as therapeutic agents

(e.g., to modulate FGF signaling and/or activities associated therewith). However, in the absence of such knowledge, candidate compounds may only be identified by a completely haphazard and random screening of different guidance, with no ability to determine what compounds may or may not be reasonably expected to work.

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SUMMARY OF THE INVENTION

The present invention seeks to overcome problems in the prior art by providing ternary complexes of: (a) an FGF ligand; (b) an FGF receptor; and (c) a heparin agonist or antagonist, that is to a say a compound that mimics the binding of heparin and heparan sulfate to the FGF ligand and receptor. Crystalline forms of such ternary complexes are also described, and crystal structure coordinates for these forms are provided.

In particular, Applicants have discovered that small, preferably sulfated molecules such as sucrose octasulfate (SOS) and its derivatives, are able to specifically and simultaneously bind to FGF ligands and FGFR polypeptides and augment binding of an FGF ligand to its receptor. Moreover, such compounds are also able to stabilize dimers of the resulting ternary complexes, effectively promoting dimerization of the FGF-FGFR complexes. Using such ternary complexes and crystal structure coordinates thereof, it is possible to identify compounds that may modulate FGF-mediated signaling and/or activities associated with such signaling. For example, the ternary complexes of this invention may be used to identify compounds that form a dimerization incompetent ternary complex with an FGF ligand and FGF receptor. Such compounds are then expected to be useful, e.g., for inhibiting FGF-mediating signaling or an activity associated therewith. For example, compounds identified by these screening methods may be used to modulate tyrosine kinase activity of an FGF receptor, or they may modulate an activity such as mitogenesis, angiogenesis, cell growth (including tumor cell growth or tumor growth) that are associated with FGF signaling. The compounds are useful, e.g., in therapeutic methods and formulations, to treat or ameliorate disorders that are associated with FGF-signaling, including cell proliferative disorders such as cancer.

The invention also provides compounds that have novel uses as modulators of FGF-signaling or an activity mediated thereby. In preferred embodiments, the compounds are derivatives of sucrose octasulfate.

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Thus, in preferred embodiments, compounds used in the methods and compositions of the invention may have the structure:

in which R₁, R₂, R₃, R₄, R₅, R₆, R₇ and R₈ are independently benzyl, trityl or -SO₃H.

Preferably at least one of R₁, R₂, R₃, R₄, R₅, R₆, R₇ and R₈ is either benzyl or trityl.

Particularly preferred, exemplary compounds are described in the Examples, *infra*, and their structures are set forth in FIG. 8 (Structures I and II), in FIG. 9 (Structure III), in FIG. 10 (Structure IV) and in FIG. 11 (Structures V and VI).

In other preferred embodiments, compounds that may be used in the methods and compositions of this invention include cyclodextrin compounds, particularly sulfated cyclodextrin compounds and sulfonated cyclodextrin compounds. The cyclodextrin compounds used may be, e.g., an α -cyclodextrin compound, a β -cyclodextrin compound or a γ -cyclodextrin compound, with β -cyclodextrin compounds being particularly preferred.

Still other compounds may also be used in the methods and compositions of this invention, including but not limited to inositol hexasulfate and suramin and their derivatives may also be used.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGS. 1A-1B present the amino acid sequence (FIG. 1A) of an exemplary

20 FGF polypeptide, known as FGF2 (SEQ ID NO:1), along with an exemplary FGF2 nucleic
acid sequence (FIG. 1B; SEQ ID NO:2) having an open reading frame () that encodes this
FGF2 polypeptide. The FGF2 polypeptide sequence (SEQ ID NO:1) is available from
GenBank and has the Accession No. P09038 (GI:122742). The nucleic acid sequence (SEQ
ID NO:2) is also available from GenBank and has the Accession No. M17599.1 (GI:183086).

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FIGS. 2A-2B present the amino acid sequence (FIG. 2A) for an exemplary FGF receptor polypeptide, known as FGFR1 (SEQ ID NO:3), along with an exemplary FGFR1 nucleic acid sequence (FIG. 2B; SEQ ID NO:4) having an open reading frame that encodes this FGFR1 polypeptide. The FGFR1 polypeptide sequence (SEQ ID NO:3) is available from GenBank and has the Accession Number P11362 (GI:120046). The nucleic acid sequence is also available from GenBank and has the Accession No. X51803.1 (GI:31367).

FIGS. 3A-D show chromatograms obtained from aliquots of purified 1:1 molar ratios of FGF2:FGFR1 complexes (2 mg) mixed with various molar ratios of sucrose octasulfate (SOS) and analyzed on a Superdex 200 size exclusion column in 25 mM HEPES-NaOH buffer (pH 7.5) containing 150 mM NaCl. The elution positions of monomers and dimers of the FGF2:FGFR1 complexes are indicated by the letters M and D, respectively. The letter L indicates the position of free FGF2 resulting from dissociation of FGF2:FGFR1 complexes due to protein dilution during the size exclusion chromatography. FIG. 3A shows the size exclusion chromatogram for a control solution that contains no SOS. FIG. 3B shows the size exclusion chromatogram when SOS was added at a molar ratio of 1:1:0.25 FGF2:FGFR1:SOS. FIG. 3C shows the size exclusion chromatogram when SOS was added at a molar ratio of 1:1:0.5 FGF2:FGFR1:SOS. FIG. 3D shows the size exclusion chromatogram when SOS was added at a molar ratio of 1:1:1.7 FGF2:FGFR1:SOS.

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FIG. 4 graphically presents average daily counts and standard deviations of viable BaF3 cells that were transfected to stably express FGFR1 and cultured in the presence of FGF2 (50 ng/ml), either alone (\bullet), with 3 μ M heparin (×) or with SOS at a concentration of 0.1 μ M (\bigcirc), 0.5 μ M (\square), 1 μ M (\triangle), 5 μ M (\Diamond) or 10 μ M (+).

FIGS. 5A-C illustrated the crystal structure determined for the FGF2-FGFR1-SOS complex. FIG. 5A illustrates an exemplary orthorhombic space group P2₁2₁2₁ crystal of the FGF2-FGFR1-SOS complex. FIGS. 5B-C illustrate the overall structure of one of the two 2:2:2 FGF2-FGFR2-SOS dimers in the crystal's asymmetric unit. The structure illustrated in FIG. 5C is identical to the structure shown in FIG. 5B, as viewed when rotated

90° around the horizontal axis.

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FIG. 6 is a stereo view of the Fo-Fc electron density map computed after simulated annealing with SOS omitted from the atomic model. The electron density map is computed at 2.6 Å resolution and contoured at 2.6 σ.

- FIG. 7 schematically illustrates interactions between SOS, FGF2 and FGFR1 in a dimerized ternary complex of FGF2, FGFR1 and SOS. Hydrogen bonding interactions are indicated by dashed lines. Shading around the different amino acid residues indicates to which polypeptide the residue belongs: FGF2, the primary FGFR1 (i.e., the FGFR1 molecule to which FGF2 is bound) and the secondary FGFR1 molecule in the dimer.
- FIG. 8 illustrates the exemplary synthesis of two preferred SOS derivatives: 2-O-Bn sucrose heptasulfate (structure I) and 1'-O-Bn sucrose heptasulfate (structure II).

FIG. 9 illustrates the exemplary synthesis of another preferred SOS derivative: 1', 2-di-O-Bn sucrose hexasulfate (structure III).

FIG. 10 illustrates the exemplary synthesis of a third preferred sulfonated sucrose derivative: 4,6-O-isopropylidene sucrose hexasulfate (Structure IV).

FIG. 11 illustrates the exemplary synthesis of two additional preferred sulfonated sucrose derivatives: 2-O-dodecanoyl sucrose hexasulfate (Structure V) and 6'-O-hexadecanoyl sucrose hexasulfate (Structure VI).

FIG. 12 illustrates the chemical structure of suramin (Structure VII).

FIG. 13 shows chromatograms obtained from aliquots of purified 1:1 molar ratios of FGF2:FGFR1 complexes (2 mg) mixed with various molar ratios of suramin and analyzed on a Superdex 200 size exclusion column in 25 mM HEPES-NaOH buffer (pH 7.5) containing 150 mM NaCl. The elution positions of monomers and dimers of the

FGF2:FGFR1 complexes are indicated by the letters M and D, respectively. The letter L indicates the position of free FGF2 resulting from dissociation of FGF2:FGFR1 complexes due to protein dilution during the size exclusion chromatography. FIG. 13A shows the size exclusion chromatogram for a control solution that contains no suramin. FIG. 13B shows the size exclusion chromatogram when suramin was added at a molar ratio of 1:1:0.25 FGF2:FGFR1:suramin. FIG. 13C shows the size exclusion chromatogram when suramin is added at a molar ratio of 1:1:0.5 FGF2:FGFR1:suramin. FIG. 13D shows the size exclusion chromatogram when suramin is added at a molar ratio of 1:1:1 FGF2:FGFR1:suramin.

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FIG. 14 illustrates an exemplary, general structure for derivatives of a preferred class of cyclodextrin molecule, β-cyclodextrin (Structure VIII). For sulfonated cyclodextrin molecules, each R group is independently selected and is preferably either a hydrogen group (H) or a sulfonate group (SO₃) with at least one R being a sulfonated group. For sulfated cyclodextrin molecules, each R group is independently selected and is preferably either a hydrogen group (H) or a sulfate group (SH) with at least one R being a sulfate group.

FIG. 15A graphically presents average daily counts and standard deviations of viable BaF3 cells that were transfected to stably express FGFR1 and cultured in the presence of FGF1 (50 ng/ml) either alone (\Box), with 10 µg/ml heparin (\times), or with sulfonated β -cyclodextrin at concentrations of 1 µM (\triangle), 5 µM (\diamondsuit), 10 µM (\diamondsuit), or 25 µM (\blacksquare).

FIGS. 15B and 15C show immunoblots of cellular proteins from BaF3 cells that overexpress FGFR1 and were incubated with FGF1 (50 ng/ml), heparin (10 μ g/ml) and sulfonated β -cyclodextrin (5 and 25 μ M). FIG. 15B shows protein bands that were immunoprecipitated with an anti-FGFR1 monoclonal antibody and detected using labeled antibody to phosphotyrosine. FIG. 15C shows protein bands that were immunoprecipitated with monoclonal antibodies to ERK-1 and/or ERK-2, and detected with labeled antibody to phosphotyrosine.

FIGS. 16A-16B present the amino acid sequence (FIG. 16A) of a second exemplary FGF polypeptide, known as FGF1 (SEQ ID NO:5), along with an exemplary FGF1

nucleic acid sequence (FIG. 16B; SEQ ID NO:6) having an open reading frame (nucleotides 142-609) that encodes this FGF1 polypeptide. The FGF1 polypeptide sequence (SEQ ID NO:5) is available from GenBank and has the Accession No. NP_000791 (GI:4503697). The nucleic acid sequence (SEQ ID NO:6) is also available from GenBank and has the Accession No. NM_000800 (GI:15055546).

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DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to a particular family or class of polypeptides, referred to herein as fibroblast growth factor (FGF) polypeptides or as FGF ligands. The FGF ligands of the invention bind to a particular family or class of receptor polypeptides, that are referred to herein as FGF receptors (FGFR). Briefly, and without being limited to any particular theory or mechanism of action, the FGF ligands are believed to mediate cell signaling by specifically binding to FGFR polypeptides. Upon binding to an FGF ligand, the FGFR polypeptide then binds to a second FGFR molecule and, more preferably, binds to a second FGFR molecule that has also bound to an FGF ligand, to form a dimer complex, and a tyrosine kinase activity of the receptor is then activated. In particular, upon forming the dimer complex biological activities (such as mitogenesis, angiogenesis and/or tumor growth) that are associated with FGF signaling may be activated and/or increased.

Under normal physiological conditions, heparan sulfate proteoglycans (HSPG) are also required to promote ligand binding and/or dimerization by FGFR. In particular, and again without being limited to any particular theory or mechanism of action, heparin and HSPGs are believed to bind to the FGF ligand and its receptor, and thereby stabilize the FGF ligand-receptor complex. Moreover, the HSPG (e.g., heparin) is also believed to interact with a second FGFR molecule, thereby promoting FGFR dimerization. More specifically, it is understood that, under normal physiological conditions FGF ligand, FGFR and heparin bind to each other to form a 1:1:1 ternary complex; i.e., a complex consisting essentially of one FGF ligand molecule, one FGFR molecule, and one heparin molecule (referred to herein as the "ternary complex" or as the FGF:FGFR:heparin complex). This ternary complex is understood to form stable dimers, by binding to a second ternary complex, under normal physiological conditions, thereby activating the FGF receptor(s).

Applicants have discovered, as demonstrated in the Examples infra, that small,

sulfated molecules may also form ternary complexes with an FGF receptor and its ligand. In particular, the Examples, *infra*, describe experiments in which sucrose octasulfate (SOS) forms a 1:1:1 ternary complex with an FGF ligand and receptor. Thus, these experiments demonstrate that small molecules such as SOS are able to act in place of heparin to stabilize binding of an FGF ligand to its receptor. Moreover, the experiments further demonstrate that SOS also stabilizes dimerization of the FGF receptor.

The Examples, *infra*, describe additional experiments demonstrating that other small molecules, particularly suramin, are also capable of forming 1:1:1 ternary complexes with an FGF ligand and receptor and, moreover, show that these molecules may function as antagonist of FGF-mediating signaling. Specifically, the experiments show that compounds such as suramin actually induce the formation of FGF - FGFR dimers that are signaling incompetent.

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The Experiments described in the Examples, *infra*, additionally provide a three-dimensional structure, determined by X-ray crystallography, for a dimeric 2:2:2 FGF2:FGFR1:SOS complex (coordinates for this structure are provided in the Appendix, *infra*). This structure reveals particular interactions between sulfate groups of the SOS and amino acid residues of FGF and FGFR. These interactions are involved in the stabilization of (1) complexes between the FGF ligand and its receptor (more specifically, the stabilization of a 1:1:1 FGF:FGFR:SOS ternary complex); and (2) FGFR dimers (more specifically, stabilization of the ternary complex dimers).

For example, hydrogen-bonding interactions are described in Example 4, *infra*, between sulfate groups of the SOS molecule, and amino acid residues lysine 163 and lysine 177 of FGFR1. Hydrogen bonding interactions are also described between sulfate groups of SOS, and amino acid residues lysine 26 and lysine 135 of FGF2. Without being limited to any particular theory or mechanism of action, these hydrogen bonding interactions are believed to be involved in the stabilization of the FGF2:FGFR1:SOS ternary complex. Other hydrogen-bonding interactions are also described between sulfate groups of the SOS molecule, and amino acid residues lysine 207, glycine 205 and aspartic acid 218 of the second FGFR1 molecule in the dimer. Thus, these other hydrogen bonding interactions are expected to be involved in stabilization of dimers of the ternary complex.

Accordingly, the present invention relates to and provides a three dimensional

(i.e. "tertiary") structure for a ternary complex (preferably a dimerized ternary complex) of (i) an FGF ligand, (ii) an FGF receptor, and (iii) a small, preferably sulfated molecule that promotes formation and/or dimerization of such a ternary complex. For example, coordinates for an exemplary structure, which is a ternary complex of FGF2:FGFR1:SOS, are provided in the Appendix, *infra*. In preferred embodiments, the small molecule is SOS or a derivative thereof. However, the skilled artisan will appreciate that other small molecules, particularly sulfated molecules, may be used, such as inositol hexasulfate, sulfated β-cyclodextrin and suramin. The invention also relates to and provides crystals comprising an above-described ternary complex which are of suitable quality and therefore useful for determining the three dimensional structure of such a complex.

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The crystals and structure of the present invention are useful, e.g., for identifying other compounds that may bind to an FGF ligand and/or its receptor and therefore modulate their activity. For example, using computer modeling algorithms and other techniques well known in the art, a user may readily use the structure provided here to identify other compounds that are expected to similarly bind to an FGF ligand and/or its receptor. Another aspect of the invention therefore involves the use of the above-mentioned structures and/or crystals to identify other compounds that interact with an FGF ligand and/or its receptor, and which may be useful, e.g., as antagonist or agonist of FGF-mediated signaling.

A skilled user may identify compounds that form or may be expected to form stabilizing interactions in a ternary complex with an FGF ligand and its receptor. In one preferred aspect, such compounds may be ones that do not form (or are not expected to form) stabilizing interactions with another ternary complex or, more specifically, with another FGF receptor. Such compounds would then be expected to inhibit dimerization of an FGF receptor, and may be used, e.g., as antagonist of an FGF receptor and/or to inhibit FGF mediated signaling and effects thereof. In another preferred aspect of such methods, the compounds identified may be ones that form (or are expected to form) improved interactions with either an FGF ligand or an FGF receptor in a ternary complex, or with a second FGF receptor (i.e., in a dimer). Such improved interactions might be, for example, hydrogen bonding or other interactions that may be either stronger or more specific that those observed for another compound (for example, stronger or more specific than interactions observed for

heparin or for SOS). Compounds identified in this aspect of the invention may be expected to bind more strongly and/or more specifically with and FGF ligand and its receptor, and may also be expected to bind more strongly and/or specifically with a second FGFR molecule to form dimers. Thus, the compounds identified in this second aspect may be useful, e.g., as agonists to increase activation of an FGF receptor and/or an activity associated therewith.

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Classes of compounds that may be identified by such screening assays include, but are not limited to, small molecules (e.g., organic or inorganic molecules which are less than about 2 kDa in molecular weight, are more preferably less than about 1 kDa in molecular weight, and/or are able to cross the blood-brain barrier and affect FGF-signaling or activities associated therewith) as well as macromolecules (e.g., molecules greater than about 2 kDa in molecular weight). Compounds identified by these screening assays may also include peptides and polypeptides. Examples of such compounds (including peptides) include but are not limited to: soluble peptides; fusion peptide members of combinatorial libraries (such as ones described by Lam et al., Nature 1991, 354:82-84; and by Houghten et al., Nature 1991, 354:84-86); members of libraries derived by combinatorial chemistry, such as molecular libraries of D- and/or L-configuration amino acids; phosphopeptides, such as members of random or partially degenerate, directed phosphopeptide libraries (see, e.g., Songyang et al., Cell 1993, 72:767-778); antibodies, including but not limited to polyclonal, monoclonal, humanized, anti-idiotypic, chimeric or single chain antibodies; antibody fragments, including but not limited to Fab, F(ab')2, Fab expression library fragments, and epitope-binding fragments thereof.

In preferred embodiments, the compounds identified in such methods are sulfated saccharides, preferably disaccharides such as sucrose octasfulate (SOS), and their derivatives. However, other small, sulfated compounds such as sulfated inositols, sulfated cyclodextrins and their derivatives may also be used. Particular exemplary compounds may include myo-inositol hexasulfate, sulfated β-cyclodextrin, and their derivatives, and suramin. Indeed, a skilled artisan will appreciate that any compound that may be modified with an FGF ligand-receptor complex (e.g., using routine computer modeling algorithms) may be used in the screening methods described here. The methods, therefore, are not limited to the particular compounds that are described in this application only to illustrate the invention.

Definitions

The terms used in this specification generally have their ordinary meanings in the art, within the context of this invention and in the specific context where each term is used. Certain terms are discussed below, or elsewhere in the specification, to provide additional guidance to the practitioner in describing the compositions and methods of the invention and how to make and use them.

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General Definitions. As used herein, the term "isolated" means that the referenced material is removed from the environment in which it is normally found. Thus, an isolated biological material can be free of cellular components, i.e., components of the cells in which the material is found or produced. In the case of nucleic acid molecules, an isolated nucleic acid includes a PCR product, an isolated mRNA, a cDNA, or a restriction fragment. In another embodiment, an isolated nucleic acid is preferably excised from the chromosome in which it may be found, and more preferably is no longer joined to non-regulatory, noncoding regions, or to other genes, located upstream or downstream of the gene contained by the isolated nucleic acid molecule when found in the chromosome. In yet another embodiment, the isolated nucleic acid lacks one or more introns. Isolated nucleic acid molecules include sequences inserted into plasmids, cosmids, artificial chromosomes, and the like. Thus, in a specific embodiment, a recombinant nucleic acid is an isolated nucleic acid. An isolated protein may be associated with other proteins or nucleic acids, or both, with which it associates in the cell, or with cellular membranes if it is a membrane-associated protein. An isolated organelle, cell, or tissue is removed from the anatomical site in which it is found in an organism. An isolated material may be, but need not be, purified.

The term "purified" as used herein refers to material that has been isolated under conditions that reduce or eliminate the presence of unrelated materials, *i.e.*, contaminants, including native materials from which the material is obtained. For example, a purified protein is preferably substantially free of other proteins or nucleic acids with which it is associated in a cell; a purified nucleic acid molecule is preferably substantially free of proteins or other unrelated nucleic acid molecules with which it can be found within a cell. As used herein, the term "substantially free" is used operationally, in the context of analytical testing of the material. Preferably, purified material substantially free of contaminants is at

least 50% pure; more preferably, at least 90% pure, and more preferably still at least 99% pure. Purity can be evaluated by chromatography, gel electrophoresis, immunoassay, composition analysis, biological assay, and other methods known in the art.

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Methods for purification are well-known in the art.. For example, nucleic acids can be purified by precipitation, chromatography (including preparative solid phase chromatography, oligonucleotide hybridization, and triple helix chromatography), ultracentrifugation, and other means. Polypeptides and proteins can be purified by various methods including, without limitation, preparative disc-gel electrophoresis, isoelectric focusing, HPLC, reversed-phase HPLC, gel filtration, ion exchange and partition chromatography, precipitation and salting-out chromatography, extraction, and countercurrent distribution. For some purposes, it is preferable to produce the polypeptide in a recombinant system in which the protein contains an additional sequence tag that facilitates purification, such as, but not limited to, a polyhistidine sequence, or a sequence that specifically binds to an antibody, such as FLAG and GST. The polypeptide can then be purified from a crude lysate of the host cell by chromatography on an appropriate solid-phase matrix. Alternatively, antibodies produced against the protein or against peptides derived therefrom can be used as purification reagents. Cells can be purified by various techniques, including centrifugation, matrix separation (e.g., nylon wool separation), panning and other immunoselection techniques, depletion (e.g., complement depletion of contaminating cells), and cell sorting (e.g., fluorescence activated cell sorting [FACS]). Other purification methods are possible. A purified material may contain less than about 50%, preferably less than about 75%, and most preferably less than about 90%, of the cellular components with which it was originally associated. The "substantially pure" indicates the highest degree of purity which can be achieved using conventional purification techniques known in the art.

A "sample" as used herein refers to a biological material which can be tested, e.g., for the presence of an FGF polypeptide or FGF nucleic acid or, alternatively, for the presence of an FGFR polypeptide or nucleic acid (e.g., to identify cells that specifically express either FGF or FGFR). Such samples can be obtained from any source, including tissue, blood and blood cells, including circulating hematopoietic stem cells (for possible detection of protein or nucleic acids), plural effusions, cerebrospinal fluid (CSF), ascites fluid, and cell culture. In preferred embodiments samples are obtained from bone marrow.

Non-human animals include, without limitation, laboratory animals such as mice, rats, rabbits, hamsters, guinea pigs, etc.; domestic animals such as dogs and cats; and, farm animals such as sheep, goats, pigs, horses, and cows.

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In preferred embodiments, the terms "about" and "approximately" shall generally mean an acceptable degree of error for the quantity measured given the nature or precision of the measurements. Typical, exemplary degrees of error are within 20 percent (%), preferably within 10%, and more preferably within 5% of a given value or range of values. Alternatively, and particularly in biological systems, the terms "about" and "approximately" may mean values that are within an order of magnitude, preferably within 5-fold and more preferably within 2-fold of a given value. Numerical quantities given herein are approximate unless stated otherwise, meaning that the term "about" or "approximately" can be inferred when not expressly stated.

The term "molecule" means any distinct or distinguishable structural unit of matter comprising one or more atoms, and includes, for example, polypeptides and polynucleotides.

The term "therapeutically effective dose" refers to that amount of a compound or compositions that is sufficient to result in a desired activity.

The phrase "pharmaceutically acceptable" refers to molecular entities and compositions that are physiologically tolerable and do not typically produce an allergic or similar untoward reaction (for example, gastric upset, dizziness and the like) when administered to an individual. Preferably, and particularly where a vaccine is used in humans, the term "pharmaceutically acceptable" may mean approved by a regulatory agency (for example, the U.S. Food and Drug Agency) or listed in a generally recognized pharmacopeia for use in animals (for example, the U.S. Pharmacopeia).

The term "carrier" refers to a diluent, adjuvant, excipient, or vehicle with which a compound is administered. Sterile water or aqueous saline solutions and aqueous dextrose and glycerol solutions are preferably employed as carriers, particularly for injectable solutions. Exemplary suitable pharmaceutical carriers are described in "Reminington's Pharmaceutical Sciences" by E.W. Martin.

Molecular Biology Definitions. In accordance with the present invention,

there may be employed conventional molecular biology, microbiology and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See, for example, Sambrook, Fitsch & Maniatis, Molecular Cloning: A Laboratory Manual, Second Edition (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York (referred to herein as "Sambrook et al., 1989"); DNA Cloning: A Practical Approach, Volumes I and II (D.N. Glover ed. 1985); Oligonucleotide Synthesis (M.J. Gait ed. 1984); Nucleic Acid Hybridization (B.D. Hames & S.J. Higgins, eds. 1984); Animal Cell Culture (R.I. Freshney, ed. 1986); Immobilized Cells and Enzymes (IRL Press, 1986); B.E. Perbal, A Practical Guide to Molecular Cloning (1984); F.M. Ausubel et al. (eds.), Current Protocols in Molecular Biology, John Wiley & Sons, Inc. (1994).

The term "polymer" means any substance or compound that is composed of two or more building blocks ('mers') that are repetitively linked together. For example, a "dimer" is a compound in which two building blocks have been joined together; a "trimer" is a compound in which three building blocks have been joined together; etc.

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The term "polynucleotide" or "nucleic acid molecule" as used herein refers to a polymeric molecule having a backbone that supports bases capable of hydrogen bonding to typical polynucleotides, wherein the polymer backbone presents the bases in a manner to permit such hydrogen bonding in a specific fashion between the polymeric molecule and a typical polynucleotide (e.g., single-stranded DNA). Such bases are typically inosine, adenosine, guanosine, cytosine, uracil and thymidine. Polymeric molecules include "double stranded" and "single stranded" DNA and RNA, as well as backbone modifications thereof (for example, methylphosphonate linkages).

Thus, a "polynucleotide" or "nucleic acid" sequence is a series of nucleotide bases (also called "nucleotides"), generally in DNA and RNA, and means any chain of two or more nucleotides. A nucleotide sequence frequently carries genetic information, including the information used by cellular machinery to make proteins and enzymes. The terms include genomic DNA, cDNA, RNA, any synthetic and genetically manipulated polynucleotide, and both sense and antisense polynucleotides. This includes single- and double-stranded molecules; *i.e.*, DNA-DNA, DNA-RNA, and RNA-RNA hybrids as well as "protein nucleic acids" (PNA) formed by conjugating bases to an amino acid backbone. This also includes

nucleic acids containing modified bases, for example, thio-uracil, thio-guanine and fluorouracil.

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The polynucleotides herein may be flanked by natural regulatory sequences, or may be associated with heterologous sequences, including promoters, enhancers, response elements, signal sequences, polyadenylation sequences, introns, 5'- and 3'-non-coding regions and the like. The nucleic acids may also be modified by many means known in the art. Nonlimiting examples of such modifications include methylation, "caps", substitution of one or more of the naturally occurring nucleotides with an analog, and internucleotide modifications such as, for example, those with uncharged linkages (e.g., methyl phosphonates, phosphotriesters, phosphoroamidates, carbamates, etc.) and with charged linkages (e.g., phosphorothioates, phosphorodithioates, etc.). Polynucleotides may contain one or more additional covalently linked moieties, such as proteins (e.g., nucleases, toxins, antibodies, signal peptides, poly-L-lysine, etc.), intercalators (e.g., acridine, psoralen, etc.), chelators (e.g., metals, radioactive metals, iron, oxidative metals, etc.) and alkylators to name a few. The polynucleotides may be derivatized by formation of a methyl or ethyl phosphotriester or an alkyl phosphoramidite linkage. Furthermore, the polynucleotides herein may also be modified with a label capable of providing a detectable signal, either directly or indirectly. Exemplary labels include radioisotopes, fluorescent molecules, biotin and the like. Other non-limiting examples of modification which may be made are provided, below, in the description of the present invention.

A "polypeptide" is a chain of chemical building blocks called amino acids that are linked together by chemical bonds called "peptide bonds". The term "protein" refers to polypeptides that contain the amino acid residues encoded by a gene or by a nucleic acid molecule (e.g., an mRNA or a cDNA) transcribed from that gene either directly or indirectly. Optionally, a protein may lack certain amino acid residues that are encoded by a gene or by an mRNA. For example, a gene or mRNA molecule may encode a sequence of amino acid residues on the N-terminus of a protein (i.e., a signal sequence) that is cleaved from, and therefore may not be part of, the final protein. A protein or polypeptide, including an enzyme, may be a "native" or "wild-type", meaning that it occurs in nature; or it may be a "mutant", "variant" or "modified", meaning that it has been made, altered, derived, or is in some way different or changed from a native protein or from another mutant.

A "ligand" is, broadly speaking, any molecule that binds to another molecule. In preferred embodiments, the ligand is either a soluble molecule or the smaller of the two molecule or both. The other molecule is referred to as a "receptor". In preferred embodiments, both a ligand and its receptor are molecules (preferably proteins or polypeptides) produced by cells. Preferably, a ligand is a soluble molecule and the receptor is an integral membrane protein (i.e., a protein expressed on the surface of a cell). In a particularly preferred embodiment of the invention the ligand is a fibroblast growth factor (FGF) and the receptor is a fibroblast growth factor receptor (FGFR).

The binding of a ligand to its receptor is frequently a step of signal transduction with a cell. For example, in preferred embodiments where a ligand is an FGF polypeptide and a receptor is an FGFR polypeptide, the binding of FGF to the FGFR polypeptide may lead to activation of a tyrosine kinase activity within the FGFR polypeptide. Activation of the tyrosine kinase activity may, in turn, initiate other activities associated with FGF signaling, including but not limited to mitogenesis and angiogensis. Other exemplary ligand-receptor interactions include, but are not limited to, binding of a hormone to a hormone receptor (for example, the binding of estrogen to the estrogen receptor) and the binding of a neurotransmitter to a receptor on the surface of a neuron.

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"Amplification" of a polynucleotide, as used herein, denotes the use of polymerase chain reaction (PCR) to increase the concentration of a particular DNA sequence within a mixture of DNA sequences. For a description of PCR see Saiki et al., Science 1988, 239:487.

"Chemical sequencing" of DNA denotes methods such as that of Maxam and Gilbert (Maxam-Gilbert sequencing; see Maxam & Gilbert, *Proc. Natl. Acad. Sci. U.S.A.* 1977, 74:560), in which DNA is cleaved using individual base-specific reactions.

"Enzymatic sequencing" of DNA denotes methods such as that of Sanger (Sanger et al., Proc. Natl. Acad. Sci. U.S.A. 1977, 74:5463) and variations thereof well known in the art, in a single-stranded DNA is copied and randomly terminated using DNA polymerase.

A "gene" is a sequence of nucleotides which code for a functional "gene

30 product". Generally, a gene product is a functional protein. However, a gene product can
also be another type of molecule in a cell, such as an RNA (e.g., a tRNA or a rRNA). For the

purposes of the present invention, a gene product also refers to an mRNA sequence which may be found in a cell. For example, measuring gene expression levels according to the invention may correspond to measuring mRNA levels. A gene may also comprise regulatory (i.e., non-coding) sequences as well as coding sequences. Exemplary regulatory sequences include promoter sequences, which determine, for example, the conditions under which the gene is expressed. The transcribed region of the gene may also include untranslated regions including introns, a 5'-untranslated region (5'-UTR) and a 3'-untranslated region (3'-UTR).

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A "coding sequence" or a sequence "encoding" an expression product, such as a RNA, polypeptide, protein or enzyme, is a nucleotide sequence that, when expressed, results in the production of that RNA, polypeptide, protein or enzyme; *i.e.*, the nucleotide sequence "encodes" that RNA or it encodes the amino acid sequence for that polypeptide, protein or enzyme.

A "promoter sequence" is a DNA regulatory region capable of binding RNA polymerase in a cell and initiating transcription of a downstream (3' direction) coding sequence. For purposes of defining the present invention, the promoter sequence is bounded at its 3' terminus by the transcription initiation site and extends upstream (5' direction) to include the minimum number of bases or elements necessary to initiate transcription at levels detectable above background. Within the promoter sequence will be found a transcription initiation site (conveniently found, for example, by mapping with nuclease S1), as well as protein binding domains (consensus sequences) responsible for the binding of RNA polymerase.

A coding sequence is "under the control of" or is "operatively associated with" transcriptional and translational control sequences in a cell when RNA polymerase transcribes the coding sequence into RNA, which is then trans-RNA spliced (if it contains introns) and, if the sequence encodes a protein, is translated into that protein.

The term "express" and "expression" means allowing or causing the information in a gene or DNA sequence to become manifest, for example producing RNA (such as rRNA or mRNA) or a protein by activating the cellular functions involved in transcription and translation of a corresponding gene or DNA sequence. A DNA sequence is expressed by a cell to form an "expression product" such as an RNA (e.g., a mRNA or a rRNA) or a protein. The expression product itself, e.g., the resulting RNA or protein, may

also said to be "expressed" by the cell.

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The term "transfection" means the introduction of a foreign nucleic acid into a cell. The term "transformation" means the introduction of a "foreign" (i.e., extrinsic or extracellular) gene, DNA or RNA sequence into a host cell so that the host cell will express the introduced gene or sequence to produce a desired substance, in this invention typically an RNA coded by the introduced gene or sequence, but also a protein or an enzyme coded by the introduced gene or sequence may also be called a "cloned" or "foreign" gene or sequence, may include regulatory or control sequences (e.g., start, stop, promoter, signal, secretion or other sequences used by a cell's genetic machinery). The gene or sequence may include nonfunctional sequences or sequences with no known function. A host cell that receives and expresses introduced DNA or RNA has been "transformed" and is a "transformant" or a "clone". The DNA or RNA introduced to a host cell can come from any source, including cells of the same genus or species as the host cell or cells of a different genus or species.

The terms "vector", "cloning vector" and "expression vector" mean the vehicle by which a DNA or RNA sequence (e.g., a foreign gene) can be introduced into a host cell so as to transform the host and promote expression (e.g., transcription and translation) of the introduced sequence. Vectors may include plasmids, phages, viruses, etc. and are discussed in greater detail below.

A "cassette" refers to a DNA coding sequence or segment of DNA that codes for an expression product that can be inserted into a vector at defined restriction sites. The cassette restriction sites are designed to ensure insertion of the cassette in the proper reading frame. Generally, foreign DNA is inserted at one or more restriction sites of the vector DNA, and then is carried by the vector into a host cell along with the transmissible vector DNA. A segment or sequence of DNA having inserted or added DNA, such as an expression vector, can also be called a "DNA construct." A common type of vector is a "plasmid", which generally is a self-contained molecule of double-stranded DNA, usually of bacterial origin, that can readily accept additional (foreign) DNA and which can readily introduced into a suitable host cell. A large number of vectors, including plasmid and fungal vectors, have been described for replication and/or expression in a variety of eukaryotic and prokaryotic hosts. The term "host cell" means any cell of any organism that is selected, modified,

transformed, grown or used or manipulated in any way for the production of a substance by the cell. For example, a host cell may be one that is manipulated to express a particular gene, a DNA or RNA sequence, a protein or an enzyme. Host cells can further be used for screening or other assays that are described *infra*. Host cells may be cultured *in vitro* or one or more cells in a non-human animal (e.g., a transgenic animal or a transiently transfected animal).

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The term "expression system" means a host cell and compatible vector under suitable conditions, e.g. for the expression of a protein coded for by foreign DNA carried by the vector and introduced to the host cell. Common expression systems include E. coli host cells and plasmid vectors, insect host cells such as Sf9, Hi5 or S2 cells and Baculovirus vectors, Drosophila cells (Schneider cells) and expression systems, and mammalian host cells and vectors.

The term "heterologous" refers to a combination of elements not naturally occurring. For example, the present invention includes chimeric RNA molecules that comprise an rRNA sequence and a heterologous RNA sequence which is not part of the rRNA sequence. In this context, the heterologous RNA sequence refers to an RNA sequence that is not naturally located within the ribosomal RNA sequence. Alternatively, the heterologous RNA sequence may be naturally located within the ribosomal RNA sequence, but is found at a location in the rRNA sequence where it does not naturally occur. As another example, heterologous DNA refers to DNA that is not naturally located in the cell, or in a chromosomal site of the cell. Preferably, heterologous DNA includes a gene foreign to the cell. A heterologous expression regulatory element is a regulatory element operatively associated with a different gene that the one it is operatively associated with in nature.

The terms "mutant" and "mutation" mean any detectable change in genetic material, e.g., DNA, or any process, mechanism or result of such a change. This includes gene mutations, in which the structure (e.g., DNA sequence) of a gene is altered, any gene or DNA arising from any mutation process, and any expression product (e.g., RNA, protein or enzyme) expressed by a modified gene or DNA sequence. The term "variant" may also be used to indicate a modified or altered gene, DNA sequence, RNA, enzyme, cell, etc.; i.e., any kind of mutant. For example, the present invention relates to altered or "chimeric" RNA molecules that comprise an rRNA sequence that is altered by inserting a heterologous RNA

sequence that is not naturally part of that sequence or is not naturally located at the position of that rRNA sequence. Such chimeric RNA sequences, as well as DNA and genes that encode them, are also referred to herein as "mutant" sequences.

"Sequence-conservative variants" of a polynucleotide sequence are those in which a change of one or more nucleotides in a given codon position results in no alteration in the amino acid encoded at that position.

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"Function-conservative variants" of a polypeptide or polynucleotide are those in which a given amino acid residue in the polypeptide, or the amino acid residue encoded by a codon of the polynucleotide, has been changed or altered without altering the overall conformation and function of the polypeptide. For example, function-conservative variants may include, but are not limited to, replacement of an amino acid with one having similar properties (for example, polarity, hydrogen bonding potential, acidic, basic, hydrophobic, aromatic and the like). Amino acid residues with similar properties are well known in the art, For example, the amino acid residues arginine, histidine and lysine are hydrophilic, basic amino acid residues and may therefore be interchangeable. Similar, the amino acid residue isoleucine, which is a hydrophobic amino acid residue, may be replaced with leucine, methionine or valine. Such changes are expected to have little or no effect on the apparent molecular weight or isoelectric point of the polypeptide. Amino acid residues other than those indicated as conserved may also differ in a protein or enzyme so that the percent protein or amino acid sequence similarity (e.g., percent identity or homology) between any two proteins of similar function may vary and may be, for example, from 70% to 99% as determined according to an alignment scheme such as the Cluster Method, wherein similarity is based on the MEGALIGN algorithm. "Function-conservative variants" of a given polypeptide also include polypeptides that have at least 60% amino acid sequence identity to the given polypeptide as determined, e.g., by the BLAST or FASTA algorithms. Preferably, function-conservative variants of a given polypeptide have at least 75%, more preferably at least 85% and still more preferably at least 90% amino acid sequence identity to the given polypeptide and, preferably, also have the same or substantially similar properties (e.g., of molecular weight and/or isoelectric point) or functions (e.g., biological functions or activities) as the native or parent polypeptide to which it is compared.

Thus, for example, in particular embodiments wherein the polypeptides are

FGFR polypeptides, function-conservative variants may not only have between at least 75% and at least 90% amino acid sequence identity to a given FGFR, but preferably also have similar properties, such as conserved domains (e.g., as in a D1, D2 or D3 domain, described supra) and/or similar biological function or activities, such as a tyrosine kinase activity and/or the ability to stimulate activities associated with FGF signaling (e.g., mitogenesis or angiogenesis).

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Similarly, in embodiments wherein a polypeptide is an FGF ligand, function-conservative variants may not only have between at least 75% and at least 90% amino acid sequence identity to a given FGF, but preferably also have similar properties. For example, a function-conservative variant of an FGF ligand preferably binds to the same FGF receptor as the FGF ligand (preferably, but not necessarily with the same or a similar affinity; e.g., preferably with at least 50% of the binding affinity, more preferably with at least 70% of the binding affinity, and still more preferably with at least 80% or at least 90% of the binding affinity). Preferably, by binding to the FGFR polypeptide, a function-conservative variant will also stimulate a same biological function or activity that is associated with binding of the FGF ligand to the receptor, including any of the functions or activities described, supra, for an FGF receptor.

The term "homologous", in all its grammatical forms and spelling variations, refers to the relationship between two proteins that possess a "common evolutionary origin", including proteins from superfamilies (e.g., the immunoglobulin superfamily) in the same species of organism, as well as homologous proteins from different species of organism (for example, myosin light chain polypeptide, etc.; see, Reeck et al., Cell 1987, 50:667). Homologous proteins of the invention therefore include various FGF proteins and polypeptides derived from the same species of organism (i.e., the FGF family of polypeptides, including FGF1-FGF22), and also FGF proteins and polypeptides derived from different species of organisms. Similarly, homologous proteins of the invention also include various FGFR proteins and polypeptides derived from the same species (i.e., the FGFR family, including FGFR1-4) or from different species of organisms.

Such proteins (and their encoding nucleic acids) have sequence homology, as reflected by their sequence similarity, whether in terms of percent identity or by the presence of specific residues or motifs and conserved positions. For instance, referring again to

particular embodiments where homologous polypeptides are FGF and/or FGFR polypeptides, homologous polypeptides in either the same or in closely related species of organisms (for example, between mammals such as mice and humans) typically share greater than 50% sequence identity, more preferably share at least about 60 to 65% sequence identity, and still more preferably share at least about 75% to 80% sequence identity. Homologous polypeptides between closely related species of organisms may also be cross reactive in both species of organisms. For example, an FGF from one species of organism may bind to and/or activate an FGF receptor polypeptide from a different species of organism and, moreover, an FGF receptor from a first species of organism may stimulate a activity associated with FGF signalling (e.g., mitogenesis or angiogenesis) in a cell from a different species of organism (for example, when the heterologous FGFR polypeptide is recombinantly expressed in that cell).

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By contrast, FGF and/or FGFR polypeptides between more divergent species of organisms share less sequence identity and generally are not cross reactive in both species. For example, homologous polypeptides between divergent species of organisms typically share less than 50% sequence identity, and may share only 25% sequence identity. However, homologous polypeptides between divergent species preferably share a higher level of sequence identity, such as between about 35% to 45% sequence identity.

The term "sequence similarity", in all its grammatical forms, refers to the degree of identity or correspondence between nucleic acid or amino acid sequences that may or may not share a common evolutionary origin (see, Reeck *et al.*, *Cell* 1987, 50:667). However, in common usage and in the instant application, the term "homologous", particularly when modified with an adverb such as "highly", may refer to sequence similarity and may or may not relate to a common evolutionary origin.

In specific embodiments, two nucleic acid sequences are "substantially homologous" or "substantially similar" when at least about 80%, and more preferably at least about 90% or at least about 95% of the nucleotides match over a defined length of the nucleic acid sequences, as determined by a sequence comparison algorithm known such as BLAST, FASTA, DNA Strider, CLUSTAL, etc. An example of such a sequence is an allelic or species variant of the specific genes of the present invention. Sequences that are substantially homologous may also be identified by hybridization, e.g., in a Southern hybridization

experiment under, e.g., stringent conditions as defined for that particular system.

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Similarly, in particular embodiments of the invention, two amino acid sequences are "substantially homologous" or "substantially similar" when greater than 80% of the amino acid residues are identical, or when greater than about 90% of the amino acid residues are similar (*i.e.*, are functionally identical). Preferably the similar or homologous polypeptide sequences are identified by alignment using, for example, the GCG (Genetics Computer Group, Program Manual for the GCG Package, *Version 7*, Madison Wisconsin) pileup program, or using any of the programs and algorithms described above (*e.g.*, BLAST, FASTA, CLUSTAL, *etc.*).

As used herein, the term "oligonucleotide" refers to a nucleic acid, generally of at least 10, preferably at least 15, and more preferably at least 20 nucleotides, preferably no more than 100 nucleotides, that is hybridizable to a genomic DNA molecule, a cDNA molecule, or an mRNA molecule encoding a gene, mRNA, cDNA, or other nucleic acid of interest. Oligonucleotides can be labeled, e.g., with ³²P-nucleotides or nucleotides to which a label, such as biotin or a fluorescent dye (for example, Cy3 or Cy5) has been covalently conjugated. In one embodiment, a labeled oligonucleotide can be used as a probe to detect the presence of a nucleic acid. In another embodiment, oligonucleotides (one or both of which may be labeled) can be used as PCR primers; e.g. for cloning full length or a fragment of either an FGF or an FGFR nucleic acid, or to detect the presence of nucleic acids encoding either an FGF or an FGFR polypeptide. Generally, oligonucleotides are prepared synthetically, preferably on a nucleic acid synthesizer. Accordingly, oligonucleotides can be prepared with non-naturally occurring phosphoester analog bonds, such as thioester bonds, etc.

Specific non-limiting examples of synthetic oligonucleotides envisioned for this invention include, in addition to the nucleic acid moieties described above, oligonucleotides that contain phosphorothioates, phosphotriesters, methyl phosphonates, short chain alkyl, or cycloalkyl intersugar linkages or short chain heteroatomic or heterocyclic intersugar linkages. Most preferred are those with CH₂-NH-O-CH₂, CH₂-N(CH₃)-O-CH₂, CH₂-O-N(CH₃)-CH₂, CH₂-N(CH₃)-N(CH₃)-CH₂ and O-N(CH₃)-CH₂-CH₂ backbones (where phosphodiester is O-PO₂-O-CH₂). US Patent No. 5,677,437 describes heteroaromatic olignucleoside linkages. Nitrogen linkers or groups containing nitrogen can also be used to

prepare oligonucleotide mimics (U.S. Patents Nos. 5,792,844 and 5,783,682). US Patent No. 5,637,684 describes phosphoramidate and phosphorothioamidate oligomeric compounds. Also envisioned are oligonucleotides having morpholino backbone structures (U.S. Pat. No. 5,034,506). In other embodiments, such as the peptide-nucleic acid (PNA) backbone, the phosphodiester backbone of the oligonucleotide may be replaced with a polyamide backbone, the bases being bound directly or indirectly to the aza nitrogen atoms of the polyamide backbone (Nielsen et al., Science 254:1497, 1991). Other synthetic oligonucleotides may contain substituted sugar moieties comprising one of the following at the 2' position: OH, SH, SCH₃, F, OCN, O(CH₂)_nNH₂ or O(CH₂)_nCH₃ where n is from 1 to about 10; C₁ to C₁₀ lower alkyl, substituted lower alkyl, alkaryl or aralkyl; Cl; Br; CN; CF3; OCF3; O-; S-, or Nalkyl; O-, S-, or N-alkenyl; SOCH₃; SO₂CH₃; ONO₂; NO₂; N₃; NH₂; heterocycloalkyl; heterocycloalkaryl; aminoalkylamino; polyalkylamino; substitued silyl; a fluorescein moiety; an RNA cleaving group; a reporter group; an intercalator; a group for improving the pharmacokinetic properties of an oligonucleotide; or a group for improving the pharmacodynamic properties of an oligonucleotide, and other substituents having similar properties. Oligonucleotides may also have sugar mimetics such as cyclobutyls or other carbocyclics in place of the pentofuranosyl group. Nucleotide units having nucleosides other than adenosine, cytidine, guanosine, thymidine and uridine, such as inosine, may be used in an oligonucleotide molecule.

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A nucleic acid molecule is "hybridizable" to another nucleic acid molecule, such as a cDNA, genomic DNA, or RNA, when a single stranded form of the nucleic acid molecule can anneal to the other nucleic acid molecule under the appropriate conditions of temperature and solution ionic strength (see Sambrook et al., supra). The conditions of temperature and ionic strength determine the "stringency" of the hybridization. For preliminary screening for homologous nucleic acids, low stringency hybridization conditions, corresponding to a T_m (melting temperature) of 55 °C, can be used, e.g., 5x SSC, 0.1% SDS, 0.25% milk, and no formamide; or 30% formamide, 5x SSC, 0.5% SDS). Moderate stringency hybridization conditions correspond to a higher T_m, e.g., 40% formamide, with 5x or 6x SCC. High stringency hybridization conditions correspond to the highest T_m, e.g., 50% formamide, 5x or 6x SCC. SCC is a 0.15M NaC1, 0.015M Na-citrate. Hybridization requires that the two nucleic acids contain complementary sequences, although depending on

the stringency of the hybridization, mismatches between bases are possible. The appropriate stringency for hybridizing nucleic acids depends on the length of the nucleic acids and the degree of complementation, variables well known in the art. The greater the degree of similarity or homology between two nucleotide sequences, the greater the value of T_m for hybrids of nucleic acids having those sequences. The relative stability (corresponding to higher T_m) of nucleic acid hybridizations decreases in the following order: RNA:RNA, DNA:RNA, DNA:DNA. For hybrids of greater than 100 nucleotides in length, equations for calculating T_m have been derived (see Sambrook et al., supra, 9.50-9.51). For hybridization with shorter nucleic acids, i.e., oligonucleotides, the position of mismatches becomes more important, and the length of the oligonucleotide determines its specificity (see Sambrook et al., supra, 11.7-11.8). A minimum length for a hybridizable nucleic acid is at least about 10 nucleotides; preferably at least about 15 nucleotides; and more preferably the length is at least about 20 nucleotides.

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In a specific embodiment, the term "standard hybridization conditions" refers to a T_m of 55°C, and utilizes conditions as set forth above. In a preferred embodiment, the T_m is 60°C; in a more preferred embodiment, the T_m is 65°C. In a specific embodiment, "high stringency" refers to hybridization and/or washing conditions at 68°C in 0.2XSSC, at 42°C in 50% formamide, 4XSSC, or under conditions that afford levels of hybridization equivalent to those observed under either of these two conditions.

Suitable hybridization conditions for oligonucleotides (e.g., for oligonucleotide probes or primers) are typically somewhat different than for full-length nucleic acids (e.g., full-length cDNA), because of the oligonucleotides' lower melting temperature. Because the melting temperature of oligonucleotides will depend on the length of the oligonucleotide sequences involved, suitable hybridization temperatures will vary depending upon the oligonucleotide molecules used. Exemplary temperatures may be 37 °C (for 14-base oligonucleotides), 48 °C (for 17-base oligonucleotides), 55 °C (for 20-base oligonucleotides) and 60 °C (for 23-base oligonucleotides). Exemplary suitable hybridization conditions for oligonucleotides include washing in 6x SSC/0.05% sodium pyrophosphate, or other conditions that afford equivalent levels of hybridization.

X-ray crystallography. The present invention also uses techniques of

conventional X-ray crystallography. These techniques are well known and are within the routine skill of the art. Such techniques are described more fully in the literature. See, for example, Cantor&Schimmel, Biophysical Chemistry 1980 (Vols. I-III) W. H. Freeman and Company (particularly Chapters 1- 13 in Vol. I, and Chapter 13 in Vol. II). See, also, Macromolecular Crystallography, Parts A-B (Carter&Sweet, Eds.) In: Methods Enzymol. 1997, Vols. 276-277; Jan Drenth, Principles of Protein X-Ray Crystallography (New York: Springer-Verlag, 1994).

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The term "crystal" refers, generally, to any ordered (or at least partially ordered) three-dimensional array of molecules. Preferably, the ordering of molecules within a crystal is at least sufficient to produce a sharp X-ray diffraction pattern so that the molecules' three-dimensional structure may be determined.

The molecules in a crystal may be of any type, and it will be understood that a crystal may contain molecules of only one type or may comprise a plurality of different types of molecules. In preferred embodiments, crystals of the present invention comprise at least one biomolecule, such as a protein, or a fragment thereof. Crystals of the invention may even comprise a complex or assembly of two or more proteins or other biomolecules. For example, a crystal may comprise two different proteins, such as a receptor and a ligand, or a crystal may comprise two more molecules of the same protein bound together, e.g., to form a dimer or other multimer complex. Typically, crystals that contain biological molecules such as proteins will contain other molecules as well, such molecules of solvent (e.g., water molecules) and/or salt. Other molecules such as drugs, drug candidates or compounds that bind to the protein may also be present in a crystal.

It will be understood by a skilled artisan that crystals of the invention comprises a "unit cell", or basic parallelepiped shaped block defined by vectors denoted a, b and c. The entire volume of a crystal may be constructed by the regular assembly of such blocks or "lattices". A crystal is also defined by the overall symmetry of elements (i.e., molecules) within the cell, which is referred to as the "space group." Thus, a crystal's space group is defined by symmetry relations within the molecules making up the unit cell. The "asymmetric unit" is the smallest possible unit from which the crystal structure may be generated by making use of the symmetric relations defining the space group.

The term "structure coordinates" or "structure" refers to mathematical

coordinates that define the position of atoms in a molecule or in an assembly of molecules in three-dimensional space (for example, within the asymmetric unit of a crystal). Structure coordinates may be computed or otherwise determined using any information related to the three dimensional arrangement of atoms in a molecule. However, in preferred embodiments of the invention a structure is derived from equations that are related to patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (which, in such embodiments, may also be referred to as "scattering centers") in a crystal. Typically, such diffraction data is used to calculate an "electron density" map of the crystal's asymmetric unit, and these maps are used, in turn, to establish positions of the individual atoms.

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"Heavy atom derivatization" refers to a method of producing chemically modified forms of a crystal (typically a crystal of a protein or other biopolymer), in which the crystal may be soaked in a solution containing heavy metal atom salts or organometallic compounds that can diffuse through the crystal and bind to the surface of the protein or biopolymer. The location(s) of one or more heavy meatl atoms in the crystal may then be determined by X-ray diffraction analysis of the soaked crystal, and this information may be used to facilitate construction of the three-dimension structure of the protein or other molecules contained in the crystal.

"Molecular replacement" refers to a method wherein a preliminary structure coordinates are generated for molecules in a crystal whose structure coordinates are not known. Generally, molecular replacement involves orienting and/or positioning another, preferably similar molecule (such as a homologous protein) whose structure coordinates are known. Phases for an X-ray diffraction pattern may then be determined for the preliminary structure, and these phases can then be combined with actual X-ray diffraction intensities that are observed for the crystal whose structure coordinates are not known, to determine its structure.

FGF Ligands

FGF Polypeptides. The present invention relates to polypeptides known as fibroblast growth factor (FGF) polypeptides or, alternatively, as FGF ligands. FGF polypeptides are well known in the art and have been described, e.g., by Mckeehan et al., (Progress in Nucleic Acid Research and Molecular Biology 1998, 59:135-176). See, also,

Nishimura et al., Biochim. Biophys. Acta 2000, 1492:203-206; and Yamashita et al., Biochem. Biophys. Res. Commun. 2000; 277:494-498. Structurally, all FGF's share a common core domain consisting of about 120 amino acids, which fold into three copies of four-stranded β-sheets known as a β-trefoil fold.

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The amino acid sequence of one, exemplary FGF polypeptide, known as FGF2, is set forth here in FIG. 1A and in SEQ ID NO:1. The FGF2 polypeptide sequence is also available from GenBank and has the Accession No. P09038 (GI:122742). The β-trefoil domain corresponds to approximately amino acid residues 28-152 of this FGF2 polypeptide sequence. The FGF2 amino acid sequence shown in FIG. 1A (SEQ ID NO:1) represents the "pre-cursor" form of the FGF2 polypeptide. This precursor is ordinarily processed by the cell and secreted as a "mature" FGF2 polypeptide comprising amino acid residues 10-155 of SEQ ID NO:1.

The amino acid sequence of a second exemplary FGF polypeptide known as FGF1 is also set forth here, in FIG. 16A and in SEQ ID NO:5. The FGF1 polypeptide is also known in the art as the acidic FGF or "aFGF", and its sequence is available from GenBank under the Accession No. NP_000791 (GI:4503697). The FGF1 amino acid sequence shown in FIG. 16A (SEQ ID NO:5) represents the "pre-cursor" form of the FGF1 polypeptide. This precursor is ordinarily processed by the cell and secreted as a "mature" FGF1 polypeptide comprising amino acid residues 16-155 of SEQ ID NO:5

Numerous variants, including FGF homologs and orthologs from the same and different species of organisms are also known in the art and/or may be readily identified. Such variants may also be used in the methods and compositions of this invention. For example, at least 22 homologous human FGF polypeptides, referred to as FGF1-FGF22, are believed to exist. The FGF polypeptides of the invention therefore include each of these human homologs, and also include homologous or orthologous polypeptides isolated from other species of organisms, particularly other mammalian species such as mouse or rat. Sequences that are substantially homologous to known FGF polypeptide sequences (e.g., to the FGF2 sequence shown in FIG. 1A and in SEQ ID NO:1 or to the FGF1 sequence in FIG. 16A and in SEQ ID NO:5) can be readily identified by comparing the sequences using standard software packages available in sequence data banks, including the BLAST algorithms (e.g., BLASTP, BLASTN, BLASTX, etc.), FASTA, DNA Strider, the GCG pileup

program, CLUSTAL and other such programs that are known in the art or are described herein.

Thus, for example, FGF polypeptides of the invention also include ones encoded by nucleic acids that hybridize to the complement of a nucleic acid molecule encoding an FGF polypeptide (e.g., in a Southern hybridization experiment under defined conditions). For example, in particular embodiments an FGF polypeptide may comprise an amino acid sequence encoded by nucleic acid molecules that hybridize to the complement of an FGF2 nucleic acid sequence, such as the coding sequence set forth in FIG. 1B (SEQ ID NO:2), under highly stringent conditions that comprise 50% formamide in 5x or 6x SSC. In other embodiments, the FGF polypeptide may comprise an amino acid sequence encoded by nucleic acid molecules that hybridize to a complement of an FGF2 nucleic acid sequence (e.g., the coding sequence in FIG.1B and SEQ ID NO:2) under moderately stringent hybridization conditions (for example, 40% formamide with 5x or 6x SSC), or under low stringency conditions (for example, in 5x SSC, 0.1% SDS, 0.25% milk, no formamide, 30% formamide, 5x SSC, or 0.5% SDS). Similarly, FGF polypeptides of the invention also encompass ones encoded by nucleic acids that hybridize to the complement of an FGF1 nucleic acid sequence, such as the coding sequence set forth in FIG. 16B (SEQ ID NO:6) under the same conditions.

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In still other embodiments, FGF polypeptides can also be identified by isolating homologous or variant FGF genes, e.g., by PCR using degenerate oligonucleotide primers designed on the basis of a given FGF polypeptide sequence and as described below.

or more partial or fragment FGF amino acid sequences; *i.e.* a portion or fragment of a full length FGF amino acid sequence such as the full length FGF2 sequence shown in FIG. 1A (SEQ ID NO:1) or, alternatively, a portion or fragment of the full length FGF1 sequence shown in FIG. 16A (SEQ ID NO:5). Such partial FGF polypeptides may comprise, for example, an amino acid sequence of one or more epitopes or domains of a full length FGF polypeptide, such as epitopes or domains of a full length FGF2 polypeptide set forth in FIG. 1B (SEQ ID NO:2) or, alternatively, of a full length FGF1 polypeptide set forth in FIG. 16A (SEQ ID NO:5). An epitope of an FGF polypeptide represents a site on the polypeptide against which an antibody may be produced and to which the antibody binds. Therefore,

polypeptides comprising the amino acid sequence of an FGF epitope are useful for making antibodies to the FGF polypeptide. Preferably, an epitope comprises a sequence of at least 5, more preferably at least 10, 15, 20, 25 or 50 amino acid residues in length. Thus, polypeptides of the invention that comprise epitopes of an FGF polypeptide preferably contain an amino acid sequence corresponding to at least 5, at least 10, at least 15, at least 20, at least 25 or at least 50 amino acid residues of a full length FGF polypeptide sequence. For example, in certain preferred embodiments wherein the epitope is an epitope of a full length FGF2 polypeptide (SEQ ID NO:1), an FGF polypeptide of the invention preferably comprises an amino acid sequence corresponding to at least 5, at least 10, at least 15, at least 20, at least 25 or at least 50 amino acid residues of the FGF2 sequence set forth in FIG. 1A (SEQ ID NO:1). Similarly, in embodiments where the epitope is an epitope to a full length FGF1 polypeptide (SEQ ID NO:5), an FGF polypeptide of the invention can comprise an amino acid sequence corresponding to at least 5, at least 10, at least 20, at least 25 or at least 50 amino acid residues of the FGF1 sequence set forth in FIG. 16A (SEQ ID NO:5).

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Truncated forms of an FGF polypeptide can also be provided. Such truncated forms may include an FGF polypeptide with a specific deletion of amino acid residues. For instance, in certain embodiments amino acid residues corresponding to one or more domains of a full length FGF polypeptide may be deleted from the amino acid sequence of an FGF polypeptide.

The FGF polypeptides of this invention include, in addition to naturally occurring homologs and orthologs of an FGF polypeptide such as FGF2 (SEQ ID NO:1) and FGF1 (SEQ ID NO:5), but also include analogs and derivatives of an FGF polypeptide. Such analogs and derivatives may be ones that are naturally occurring (such as allelic variants), or may be man made (such as fusion proteins). However, analogs and derivatives of an FGF polypeptide of this invention will have the same or homologous characteristics of FGF polypeptides set forth above.

An FGF chimeric or fusion polypeptide may also be prepared in which the FGF portion of the fusion polypeptide has one or more characteristics of the FGF polypeptide. Such fusion polypeptides therefore represent alternative embodiments of the FGF polypeptides of this invention. Exemplary FGF fusion polypeptides include ones which comprise a full length, derivative or truncated FGF amino acid sequence, as well as fusions

which comprise a fragment of an FGF polypeptide sequence (e.g., a fragment corresponding to an epitope or to one or more domains). Such fusion polypeptides may also comprise the amino acid sequence of a second, different polypeptide. For example, a fusion protein of the invention may comprise the amino acid sequence of a marker polypeptide; such as FLAG, a histidine tag, glutathione S-transferase (GST), or an Fc portion of an IgG. In other embodiments, an FGF polypeptide may be expressed with (e.g., fused to) a bacterial protein such as β -galactosidase. Additionally, FGF fusion polypeptides may comprise amino acid sequences that increase solubility of the polypeptide, such as thioreductase amino acid sequence, or the sequence of one or more immunoglobulin proteins (e.g., IgG1 or IgG2).

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FGF analogs or variants can also be made by altering encoding nucleic acid molecules, for example by substitutions, additions or deletions. Preferably such altered nucleic acid molecules encode functionally similar molecules (*i.e.*, molecules that perform one or more functions of an FGF ligand and/or have one or more FGF bioactivities). Thus, in a specific embodiment, an analog or variant of an FGF ligand is a function-conservative analog or variant.

Amino acid residues, other than ones that are specifically identified herein as being conserved, may differ among variants of a protein or polypeptide. Accordingly, the percentage of protein or amino acid sequence similarity between any two FGF polypeptides of similar function may vary. Typically, the percentage of protein or amino acid sequence similarity between different FGF variants may be from 70% to 99%, as determined according to an alignment scheme such as the Cluster Method and/or the MEGALIGN or GCG alignment algorithm. "Function-conservative variants" also include polypeptides that have greater than or at least 20%, or greater than or at least 25%, preferably greater than or at least 45%, more preferably greater than or at least 50, 75, 85, 90 or 95% sequence similarity to a FGF polypeptide (such as FGF2, set forth in SEQ ID NO:1 and in FIG. 1A; or, alternatively, FGF1 set forth in SEQ ID NO:5 and in FIG. 16A) or to one or more fragments or domains thereof. Preferably, such function-conservative variants also have the same or similar properties, functions or bioactivities as the native polypeptide to which they are compared. It is further noted that function-conservative variants of the present invention include, not only variants of a full length FGF polypeptide, but also include function-conservative variants of modified FGF polypeptides (e.g., truncations and deletions) and of fragments (e.g.,

corresponding to domains or epitopes) of full length FGF polypeptides.

encoded by allelic variants or mutants of an FGF nucleic acid. (described infra).

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In still other embodiments, an analog of an FGF polypeptide may be an allelic variant or mutant FGF polypeptide. The terms allelic variant and mutant, when used herein to describe a polypeptide, refer to a polypeptide encoded by an allelic variant or mutant gene.

Thus, the allelic variant and mutant FGF polypeptides of the invention are polypeptides

FGF polypeptides of the invention also include derivative FGF polypeptides, which may be phosphorylated, myristylated, methylated or otherwise chemically modified. Such derivative FGF polypeptides also include labeled variants; for example, radio-labeled with iodine, phosphorous or sulfur (see, e.g., EP 372707 B) or FGF polypeptides labeled with other detetable molecules such as, but by no means limited to, biotin, a fluorescent dye (e.g., Cy5 or Cy3), a chelating group complexed with a metal ion, a chromophore or fluorophore, a gold colloid, a particular such as a latex bead, or attached to a water soluble polymer.

Chemical modifications of a biologically active component or components of FGF nucleic acids or polypeptides may provide additional advantages under certain circumstances. See, for example, U.S. Patent No. 4,179,337 issued December 18, 1970 to Davis et al. Also, for a review see, Abuchowski et al., in Enzymes as Drugs (J.S. Holcerberg & J. Roberts, eds.) 1981, pages 367-383. A review article describing protein modification and fusion proteins is also found in Fracis, Focus on Growth Factors 1992, 3:4-10,

20 Mediscript: Mountview Court, Friern Barnet Lane, London N20, OLD, UK.

While the above, exemplary variants and analogs of FGF polypeptides are described primarily in terms of the exemplary FGF polypepide, FGF2 (set forth in FIG. 1A and SEQ ID NO:1) and FGF1 (set forth in FIG. 16A and SEQ ID NO:5), it is understood that variant FGF polypeptides of the invention include other FGF polypeptides (e.g., naturally occurring homologs and orthologs, described supra) having equivalent amino acid substitutions, deletions or insertions.

FGF nucleic acids. In general, an FGF nucleic acid molecule of the present invention comprises a nucleic acid sequence that encodes an FGF polypeptide (as defined, above, in this Subsection) or the complement of an FGF polypeptide encoding sequence. The invention also provides fragments of FGF encoding sequences and their complements, and

such sequences are also considered part of the FGF nucleic acid molecules of this invention. Thus, in one exemplary embodiment, an FGF nucleic acid molecule of the invention may encode the exemplary FGF2 polypeptide sequence set forth in FIG. 1A (SEQ ID NO:1), such as the particular FGF2 nucleic acid sequence that is depicted in FIG. 1B (i.e., SEQ ID NO:2). In another exemplary embodiment, an FGF nucleic acid of the invention may encode the eemplary FGF1 polypeptide sequence set forth in FIG. 16A (SEQ ID NO:5), such as the particular FGF1 nucleic acid sequence shown in FIG. 16B (SEQ ID NO:6).

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In still other embodiments, the FGF nucleic acid molecules of the invention comprise nucleic acid sequences that encode one or more domains of an FGF polypeptide.

The FGF nucleic acid molecules of the invention also include nucleic acids which comprise a sequence encoding one or more fragments of an FGF polypeptide. Such fragments include, for example, polynucleotides that encode an epitope of an FGF polypeptide; e.g., nucleic acids that encode a sequence of at least 5, and more preferably at least 10, 15, 20, 25 or 50 amino acid residues of an FGF polypeptide sequence (for example, of the exemplary FGF2 polypeptide sequence set forth in FIG. 1A and in SEQ ID NO:1 or, alternatively, of the exemplary FGF1 polypeptide sequence in FIG. 16A and in SEQ ID NO:5).

As explained above, numerous variant FGF polypeptides are known in the art and may be readily identified by those skilled in the art, including homologous and orthologous polypeptides from the same and different species of organism. The FGF nucleic acid molecules of the invention therefore include nucleic acid molecule comprising coding sequences for variant FGF polypeptides (including allelic variants, analogs and homologous from the same or different species), as well as nucleic acid molecule comprising coding sequences for modified FGF polypeptides (e.g., having amino acid substitutions, deletions or truncations). In preferred embodiments, such nucleic acid molecules have at least 50%, preferably at least 75% and more preferably at least 90% sequence identity to another FGF coding sequence, such as the exemplary FGF2 coding sequence set forth in FIG. 1B (SEQ ID NO:2) or, alternatively, the exemplary FGF1 coding sequence shown in FIG. 16B (SEQ ID NO:6).

In addition, the FGF nucleic acid molecules of the invention include nucleic acid molecules that hybridize to another FGF nucleic acid molecule, e.g., in a Southern blot

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assay under defined conditions. For example, in specific embodiments an FGF nucleic acid molecule of the invention comprises a nucleotide sequence which hybridizes to a complement of the exemplary FGF2 coding sequence set forth in FIG. 1B (SEQ ID NO:2) under highly stringent hybridization conditions that comprise 50% formamide and 5x or 6x SSC. In other embodiments, the nucleic acid molecules hybridize to a complement of an FGF nucleic acid sequence (e.g., to the exemplary coding sequence set forth in FIG. 1B and in SEQ ID NO:2) under moderately stringent hybridization conditions (e.g., in 5x SSC, 0.1% SDS, 0.25% milk, no formamide, 30% formamide, 5x SSC or 0.5% SDS). Similarly, an FGF nucleic acid of the invention may comprise a nucleotide sequence that hybridizes to a complement of the exemplary FGF1 coding sequence set forth in FIG. 16B (SEQ ID NO:6) under the same conditions. Alternatively, an FGF nucleic acid molecule may hybridize, under the same defined hybridization conditions, to the complement of a fragment of a nucleotide sequence encoding a full length FGF polypeptide.

In other embodiments, FGF nucleic acid molecules of the invention comprise fragments of a full length FGF nucleic acid sequence. Such nucleic acid fragments comprise a nucleotide sequence that corresponds to a sequence of at least 10 nucleotides, preferably at least 15 nucleotides and more preferably at least 20 nucleotides of a full length coding FGF nucleotide sequence. In specific embodiments, the fragments correspond to a portion (e.g., of at least 10, 15, or 20 nucleotides) of the exemplary FGF2 coding sequence shown in FIG. 1B (SEQ ID NO:2) or of the exemplary FGF1 coding sequence shown in FIG. 16B (SEQ ID NO:6). In other embodiments, an FGF nucleic acid fragment may comprise sequences of at least 10, preferably at least 15, and more preferably at least 20 nucleotides that are complementary and/or hybridize to a full length FGF coding sequence (e.g., the FGF2 coding sequence set forth in FIG. 1B and in SEQ ID NO:2, or the FGF1 coding sequence set forth in FIG. 16B and in SEQ ID NO:6) or to a fragment thereof.

Suitable hybridization conditions for such oligonucleotides are described supra, and include washing in 6x SSC/0.05% sodium pyrophosphate. Because the melting temperature of oligonucleotides will depend on the length of the oligonucleotide sequence, suitable hybridization temperatures may vary depending upon the oligonucleotide molecules used. Those skilled in the art will be able to select a suitable hybridization temperature using routine techniques described, e.g., in any of the molecular biology references cited supra.

Exemplary temperatures will be 37 °C (e.g., for 14-base oligonucleotides), 48 °C (e.g., for 17-base oligonucleotides), 55 °C (e.g., for 20-base oligonucleotides) and 60 °C (e.g., for 23-base oligonucleotides).

Nucleic acid molecules comprising such fragments are useful, for example, as oligonucleotide probes and primers (e.g., PCR primers) to detect and amplify other nucleic acid molecules encoding an FGF polypeptide, including genes that encode variant FGF polypeptides (including genes that encode homologous or orthologous FGF polypeptides from the same or different species of organism). Oligonucleotide fragments of the invention may also be used, e.g., as antisense nucleic acids, triple helix forming oligonucleotides or as ribozymes (e.g., to modulate levels of FGF gene expression or transcription in cells).

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The nucleic acid molecules of the invention also include "chimeric" FGF nucleic acid molecules. Such chimeric nucleic acid molecules are polynucleotides which comprise at least one FGF nucleic acid sequence (which may be any of the full length or partial FGF nucleic acid sequences described above), and also at least one non-FGF nucleic acid sequence. For example, the non-FGF nucleic acid sequence may be a heterologous regulatory sequence (for example, a promoter sequence) that is derived from another, non-FGF gene and is not normally associated with a naturally occurring FGF gene. A non-FGF nucleic acid sequence of the invention may also be a coding sequence of another, non-FGF polypeptide such as FLAG, a histidine tag, glutathione S-transferase (GST), hemaglutinin, β-galactosidase, thioreductase or an immunoglobulin domain or domains (for example, an Fc region). In preferred embodiments, a chimeric nucleic acid molecule of the invention encodes an FGF fusion polypeptide of the invention.

FGF nucleic acid molecules of the invention, whether genomic DNA, cDNA or otherwise, can be isolated from any source including, for example, cDNA or genomic libraries derived from a cell or cell line from an organism that has a FGF gene. In the case of cDNA libraries, such libraries are preferably derived from a cell or cell line that expresses an FGF gene. Methods for obtaining FGF genes are well known in the art, as described above (see, e.g., Sambrook et al., 1989, supra).

The DNA may be obtained by standard procedures known in the art from cloned DNA (for example, from a DNA "library"), and preferably is obtained from a cDNA library prepared from tissues with high level expression of the protein (e.g., from cells or

from tissue. In one preferred embodiment, the DNA is obtained from a "subtraction" library to enrich the library for cDNAs of genes specifically expressed by a particular cell type or under certain conditions. Use of such a subtraction library may increase the likelihood of isolating cDNA for a particular gene, such as a particular FGF gene. In still other embodiments, a library may be prepared by chemical synthesis, by cDNA cloning, or by the cloning of genomic DNA or fragments thereof purified from the desired cell (See, for example, Sambrook et al., 1989, supra; Glover, D.M. ed., 1985, DNA Cloning: A Practical Approach, MRL Press, Ltd. Oxford, U.K. Vols. I and II).

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In one embodiment, a cDNA library may be screened for an FGF nucleic acid by identifying cDNA inserts that encode a polypeptide which is homologous or substantially similar to an FGF polypeptide, such as the exemplary FGF2 polypeptide set forth in FIG. 1A (SEQ ID NO:1), the exemplary FGF1 polypeptide set forth in FIG. 16A (SEQ ID NO:5) or fragments thereof. Similarly, a cDNA library may be screened for an FGF nucleic acid by identifying cDNA inserts having a nucleic acid sequence that is homologous or substantially similar to an FGF nucleic acid sequence, such as the exemplary FGF2 nucleic acid sequence set forth in FIG. 1B (SEQ ID NO:2), the exemplary FGF1 nucleic acid sequence set forth in FIG. 16B (SEQ ID NO:6) or fragments thereof.

Clones derived from genomic DNA may contain regulatory and intron DNA regions in addition to coding regions. Clones derived from cDNA generally will not contain intron sequences. Whatever the source, the gene is preferably molecularly cloned into a suitable vector for propagation of the gene. Identification of the specific DNA fragment containing the desired FGF gene may be accomplished in a number of ways. For example, a portion of an FGF gene can be purified and labeled to prepare a labeled probe (Benton & Davis, Science 1977, 196:180; Grunstein & Hogness, Proc. Natl. Acad. Sci. U.S.A. 1975, 72:3961). Those DNA fragments with substantial homology to the probe (for example, an allelic variant from another individual, or a homologous FGF gene from the same or a different species of organism) will hybridize. In a specific embodiment, highest stringency hybridization conditions are used to identify a homologous FGF gene. However, lower (e.g., moderate) hybridization conditions may also be used.

Further selection can be carried out on the basis of the properties of the FGF gene product, e.g., if the gene encodes a protein product having the isoelectric,

electrophoretic, amino acid composition, partial or complete amino acid sequence, antibody binding activity, or ligand binding profile of a FGF polypeptide. Thus, the presence of the gene may be detected by assays based on the physical, chemical, immunological, or functional properties of its expressed product.

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Other DNA sequences which encode substantially the same amino acid sequence as a FGF gene may be used in the practice of the present invention. These include but are not limited to allelic variants, species variants, sequence conservative variants, and functional variants. In particular, the nucleic acid sequences of the invention include both "function-conservative variants" and "sequence-conservative variants". Nucleic acid substitutions may be made for example, to alter the amino acid residue encoded by a particular codon, and thereby substitute an amino acid in a FGF polypeptide for one with a particularly preferable property. For example, a Cysteine amino acid residue may be introduced at a potential site for disulfide bridges with another Cysteine amino acid residue. Conversely, an amino acid residue, for example a Serine amino acid residue, may be substituted for a Cysteine amino acid residue in an FGF polypeptide. Such substitutions may be useful, for example, to facilitate solubilization of a recombinant FGF polypeptide.

The genes encoding FGF derivatives and analogs of the invention can be produced by various methods known in the art. The manipulations which result in their production can occur at the gene or protein level. For example, the cloned FGF gene sequence can be modified by any of numerous strategies known in the art (Sambrook et al., 1989, supra). The sequence can be cleaved at appropriate sites with restriction endonuclease(s), followed by further enzymatic modification if desired, isolated, and ligated in vitro. In the production of the gene encoding a derivative or analog of FGF, care should be taken to ensure that the modified gene remains within the same translational reading frame as the original FGF gene, uninterrupted by translational stop signals, in the gene region where the desired activity is encoded.

Additionally, the FGF-encoding nucleic acid sequence can be mutated *in vitro* or *in vivo*, to create and/or destroy translation, initiation, and/or termination sequences, or to create variations in coding regions and/or form new restriction endonuclease sites or destroy preexisting ones, to facilitate further *in vitro* modification. Modifications can also be made to introduce restriction sites and facilitate cloning the FGF gene into an expression vector. Any

technique for mutagenesis known in the art can be used, including but not limited to, in vitro site-directed mutagenesis (Hutchinson, C., et al., J. Biol. Chem. 253:6551, 1978; Zoller and Smith, DNA 3:479-488, 1984; Oliphant et al., Gene 44:177, 1986; Hutchinson et al., Proc. Natl. Acad. Sci. U.S.A. 83:710, 1986), use of TAB" linkers (Pharmacia), etc. PCR techniques are preferred for site directed mutagenesis (see Higuchi, 1989, "Using PCR to Engineer DNA", in PCR Technology: Principles and Applications for DNA Amplification, H. Erlich, ed., Stockton Press, Chapter 6, pp. 61-70).

The identified and isolated gene can then be inserted into an appropriate cloning vector. A large number of vector-host systems known in the art may be used. Possible vectors include, but are not limited to, plasmids or modified viruses, but the vector system must be compatible with the host cell used. Examples of vectors include, but are not limited to, E. coli, bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid derivatives, e.g., pGEX vectors, pmal-c, pFLAG, pKK plasmids (Clonetech), pET plasmids (Novagen, Inc., Madison, WI), pRSET or pREP plasmids, pcDNA (Invitrogen, Carlsbad, CA), or pMAL plasmids (New England Biolabs, Beverly, MA), etc. The insertion into a cloning vector can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini. However, if the complementary restriction sites used to fragment the DNA are not present in the cloning vector, the ends of the DNA molecules may be enzymatically modified. Alternatively, any site desired may be produced by ligating nucleotide sequences (linkers) onto the DNA termini. These ligated linkers may comprise specific chemically synthesized oligonucleotides encoding restriction endonuclease recognition sequences.

Recombinant molecules can be introduced into host cells via transformation, transfection, infection, electroporation, etc., so that many copies of the gene sequence are generated. Preferably, the cloned gene is contained on a shuttle vector plasmid, which provides for expansion in a cloning cell, e.g., E. coli, and facile purification for subsequent insertion into an appropriate expression cell line, if such is desired. For example, a shuttle vector, which is a vector that can replicate in more than one type of organism, can be prepared for replication in both E. coli and Saccharomyces cerevisiae by linking sequences from an E. coli plasmid with sequences from the yeast 2m plasmid.

Expression of FGF polypeptides. A nucleotide sequence coding for an FGF polypeptide, for an antigenic fragment, derivative or analog of an FGF polypeptide, or for a functionally active derivative of an FGF polypeptide (including a chimeric protein) may be inserted into an appropriate expression vector, i.e., a vector which contains the necessary elements for the transcription and translation of the inserted protein-coding sequence. Thus, a nucleic acid encoding a FGF polypeptide of the invention can be operationally associated with a promoter in an expression vector of the invention. Both cDNA and genomic sequences can be cloned and expressed under control of such regulatory sequences. Such vectors can be used to express functional or functionally inactivated FGF polypeptides.

The necessary transcriptional and translational signals can be provided on a recombinant expression vector.

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Potential host-vector systems include but are not limited to mammalian or other vertebrate cell systems transfected with expression plasmids or infected with virus (e.g., vaccinia virus, adenovirus, adeno-associated virus, herpes virus, etc.); insect cell systems infected with virus (e.g., baculovirus); microorganisms such as yeast containing yeast vectors; or bacteria transformed with bacteriophage, DNA, plasmid DNA, or cosmid DNA. The expression elements of vectors vary in their strengths and specificities. Depending on the host-vector system utilized, any one of a number of suitable transcription and translation elements may be used.

Expression of a FGF polypeptide may be controlled by any promoter/enhancer element known in the art, but these regulatory elements must be functional in the host selected for expression. Promoters which may be used to control FGF gene expression include, but are not limited to, cytomegalovirus (CMV) promoter (U.S. Patent Nos. 5,385,839 and 5,168,062), the SV40 early promoter region (Benoist and Chambon, Nature 1981, 290:304-310), the promoter contained in the 3' long terminal repeat of Rous sarcoma virus (Yamamoto, et al., Cell 1980, 22:787-797), the herpes thymidine kinase promoter (Wagner et al., Proc. Natl. Acad. Sci. U.S.A. 1981, 78:1441-1445), the regulatory sequences of the metallothionein gene (Brinster et al., Nature 1982, 296:39-42); prokaryotic expression vectors such as the b-lactamase promoter (Villa-Komaroff, et al., Proc. Natl. Acad. Sci. U.S.A. 1978, 75:3727-3731), or the tac promoter (DeBoer, et al., Proc. Natl. Acad. Sci. U.S.A. 1983, 80:21-25, 1983); see also "Useful proteins from recombinant bacteria" in

Scientific American 1980, 242:74-94. Still other useful promoter elements which may be used include promoter elements from yeast or other fungi such as the Gal 4 promoter, the ADC (alcohol dehydrogenase) promoter, PGK (phosphoglycerol kinase) promoter, alkaline phosphatase promoter; and transcriptional control regions that exhibit hematopoietic tissue specificity, in particular: beta-globin gene control region which is active in myeloid cells (Mogram et al., Nature 1985, 315:338-340; Kollias et al., Cell 1986, 46:89-94), hematopoietic stem cell differentiation factor promoters, erythropoietin receptor promoter (Maouche et al., Blood 1991, 15:2557), etc.

Indeed, any type of plasmid, cosmid, YAC or viral vector may be used to prepare a recombinant nucleic acid construct which can be introduced to a cell, or to tissue, where expression of an FGF gene product is desired. Alternatively, wherein expression of a recombinant FGF gene product in a particular type of cell or tissue is desired, viral vectors that selectively infect the desired cell type or tissue type can be used.

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In another embodiment, the invention provides methods for expressing FGF polypeptides by using a non-endogenous promoter to control expression of an endogenous FGF gene within a cell. An endogenous FGF gene within a cell is an FGF gene of the present invention which is ordinarily (i.e., naturally) found in the genome of that cell. A nonendogenous promoter, however, is a promoter or other nucleotide sequence that may be used to control expression of a gene but is not ordinarily or naturally associated with the endogenous FGF gene. As an example, methods of homologous recombination may be employed (preferably using non-protein encoding FGF nucleic acid sequences of the invention) to insert an amplifiable gene or other regulatory sequence in the proximity of an endogenous FGF gene. The inserted sequence may then be used, e.g., to provide for higher levels of FGF gene expression than normally occurs in that cell, or to overcome one or more mutations in the endogenous FGF regulatory sequences which prevent normal levels of FGF gene expression. Such methods of homologous recombination are well known in the art. See, for example, International Patent Publication No. WO 91/06666, published May 16, 1991 by Skoultchi; International Patent Publication No. WO 91/099555, published July 11, 1991 by Chappel; and International Patent Publication No. WO 90/14092, published November 29, 1990 by Kucherlapati and Campbell.

Soluble forms of the protein can be obtained by collecting culture fluid, or

solubilizing inclusion bodies, e.g., by treatment with detergent, and if desired sonication or other mechanical processes, as described above. The solubilized or soluble protein can be isolated using various techniques, such as polyacrylamide gel electrophoresis (PAGE), isoelectric focusing, 2-dimensional gel electrophoresis, chromatography (e.g., ion exchange, affinity, immunoaffinity, and sizing column chromatography), centrifugation, differential solubility, immunoprecipitation, or by any other standard technique for the purification of proteins.

A wide variety of host/expression vector combinations may be employed in expressing the DNA sequences of this invention. Useful expression vectors, for example, may consist of segments of chromosomal, non-chromosomal and synthetic DNA sequences. Suitable vectors include derivatives of SV40 and known bacterial plasmids, e.g., E. coli plasmids col El, pCR1, pBR322, pMal-C2, pET, pGEX (Smith et al., Gene 1988, 67:31-40), pCR2.1 and pcDNA 3.1+ (Invitrogen, Carlsbad, California), pMB9 and their derivatives, plasmids such as RP4; phage DNAs, e.g., the numerous derivatives of phage 1, e.g., NM989, and other phage DNA, e.g., M13 and filamentous single stranded phage DNA; yeast plasmids such as the 2m plasmid or derivatives thereof; vectors useful in enkaryotic cells, such as vectors useful in insect or mammalian cells; vectors derived from combinations of plasmids and phage DNAs, such as plasmids that have been modified to employ phage DNA or other expression control sequences; and the like.

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Preferred vectors are viral vectors, such as lentiviruses, retroviruses, herpes viruses, adenoviruses, adeno-associated viruses, vaccinia virus, baculovirus, and other recombinant viruses with desirable cellular tropism. Thus, a gene encoding a functional or mutant FGF polypeptide or a domain fragment thereof can be introduced *in vivo*, *ex vivo*, or *in vitro* using a viral vector or through direct introduction of DNA. Expression in targeted tissues can be effected by targeting the transgenic vector to specific cells, such as with a viral vector or a receptor ligand, or by using a tissue-specific promoter, or both. Targeted gene delivery is described in International Patent Publication WO 95/28494, published October 1995.

Viral vectors commonly used for *in vivo* or *ex vivo* targeting and therapy procedures are DNA-based vectors and retroviral vectors. Methods for constructing and using viral vectors are known in the art (see, e.g., Miller and Rosman, BioTechniques 1992,

7:980-990). Preferably, the viral vectors are replication defective, that is, they are unable to replicate autonomously in the target cell. In general, the genome of the replication defective viral vectors which are used within the scope of the present invention lack at least one region which is necessary for the replication of the virus in the infected cell. These regions can either be eliminated (in whole or in part), be rendered non-functional by any technique known to a person skilled in the art. These techniques include the total removal, substitution (by other sequences, in particular by the inserted nucleic acid), partial deletion or addition of one or more bases to an essential (for replication) region. Such techniques may be performed in vitro (on the isolated DNA) or in situ, using the techniques of genetic manipulation or by treatment with mutagenic agents. Preferably, the replication defective virus retains the sequences of its genome which are necessary for encapsidating the viral particles.

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DNA viral vectors include an attenuated or defective DNA virus, such as but not limited to herpes simplex virus (HSV), papillomavirus, Epstein Barr virus (EBV), adenovirus, adeno-associated virus (AAV), and the like. Defective viruses, which entirely or almost entirely lack viral genes, are preferred. Defective virus is not infective after introduction into a cell. Use of defective viral vectors allows for administration to cells in a specific, localized area, without concern that the vector can infect other cells. Thus, a specific tissue can be specifically targeted. Examples of particular vectors include, but are not limited to, a defective herpes virus 1 (HSV1) vector (Kaplitt et al., Molec. Cell. Neurosci. 1991, 2:320-330), defective herpes virus vector lacking a glyco-protein L gene (Patent Publication RD 371005 A), or other defective herpes virus vectors (International Patent Publication No. WO 94/21807, published September 29, 1994; International Patent Publication No. WO 92/05263, published April 2, 1994); an attenuated adenovirus vector, such as the vector described by Stratford-Perricaudet et al. (J. Clin. Invest. 1992, 90:626-630; see also La Salle et al., Science 1993, 259:988-990); and a defective adeno-associated virus vector (Samulski et al., J. Virol. 1987, 61:3096-3101; Samulski et al., J. Virol. 1989, 63:3822-3828; Lebkowski et al., Mol. Cell. Biol. 1988, 8:3988-3996).

Various companies produce viral vectors commercially, including but by no means limited to Avigen, Inc. (Alameda, CA; AAV vectors), Cell Genesys (Foster City, CA; retroviral, adenoviral, AAV vectors, and lentiviral vectors), Clontech (retroviral and baculoviral vectors), Genovo, Inc. (Sharon Hill, PA; adenoviral and AAV vectors), Genvec

(adenoviral vectors), IntroGene (Leiden, Netherlands; adenoviral vectors), Molecular Medicine (retroviral, adenoviral, AAV, and herpes viral vectors), Norgen (adenoviral vectors), Oxford BioMedica (Oxford, United Kingdom; lentiviral vectors), Transgene (Strasbourg, France; adenoviral, vaccinia, retroviral, and lentiviral vectors) and Invitrogen (Carlbad, California).

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In another embodiment, the vector can be introduced in vivo by lipofection, as naked DNA, or with other transfection facilitating agents (peptides, polymers, etc.). Synthetic cationic lipids can be used to prepare liposomes for in vivo transfection of a gene encoding a marker (Felgner et al., Proc. Natl. Acad. Sci. U.S.A. 1987, 84:7413-7417; Felgner and Ringold, Science 1989, 337:387-388; Mackey et al., Proc. Natl. Acad. Sci. U.S.A. 1988, 85:8027-8031; Ulmer et al., Science 1993, 259:1745-1748). Useful lipid compounds and compositions for transfer of nucleic acids are described in International Patent Publications WO 95/18863 and WO 96/17823, and in U.S. Patent No. 5,459,127. Lipids may be chemically coupled to other molecules for the purpose of targeting (see, Mackey et al., Proc. Natl. Acad. Sci. U.S.A. 1988, 85:8027-8031). Targeted peptides, e.g., hormones or neurotransmitters, and proteins such as antibodies, or non-peptide molecules could be coupled to liposomes chemically. Other molecules are also useful for facilitating transfection of a nucleic acid in vivo, such as a cationic oligopeptide (e.g., International Patent Publication WO 95/21931), peptides derived from DNA binding proteins (e.g., International Patent Publication WO 96/25508), or a cationic polymer (e.g., International Patent Publication WO 95/21931).

It is also possible to introduce the vector *in vivo* as a naked DNA plasmid. Naked DNA vectors for gene therapy can be introduced into the desired host cells by methods known in the art, e.g., electroporation, microinjection, cell fusion, DEAE dextran, calcium phosphate precipitation, use of a gene gun, or use of a DNA vector transporter (see, e.g., Wu et al., J. Biol. Chem. 1992, 267:963-967; Wu and Wu, J. Biol. Chem. 1988, 263:14621-14624; Hartmut et al., Canadian Patent Application No. 2,012,311, filed March 15, 1990; Williams et al., Proc. Natl. Acad. Sci. U.S.A. 1991, 88:2726-2730). Receptor-mediated DNA delivery approaches can also be used (Curiel et al., Hum. Gene Ther. 1992, 3:147-154; Wu and Wu, J. Biol. Chem. 1987, 262:4429-4432). US Patent Nos. 5,580,859 and 5,589,466 disclose delivery of exogenous DNA sequences, free of transfection facilitating agents, in a

mammal. Recently, a relatively low voltage, high efficiency in vivo DNA transfer technique, termed electrotransfer, has been described (Mir et al., C.P. Acad. Sci. 1998, 321:893; WO 99/01157; WO 99/01158; WO 99/01175).

Preferably, for *in vivo* administration, an appropriate immunosuppressive treatment is employed in conjunction with the viral vector, e.g., adenovirus vector, to avoid immuno-deactivation of the viral vector and transfected cells. For example, immunosuppressive cytokines, such as interleukin-12 (IL-12), interferon-g (IFN-γ), or anti-CD4 antibody, can be administered to block humoral or cellular immune responses to the viral vectors (see, e.g., Wilson, Nat. Med. 1995, 1:887-889). In that regard, it is advantageous to employ a viral vector that is engineered to express a minimal number of antigens.

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FGF Receptors

FGF receptor polypeptides. The present invention relates, not only to FGF ligand polypeptides, described supra, but also to receptor polypeptides that specifically bind to an FGF polypeptide. Such receptor polypeptides are generally referred to as FGF receptor polypeptides or FGFR polyeptides.

In preferred embodiments, an FGFR polypeptide of the invention is characterized by its biological activity or activities; *i.e.*, an FGFR polypeptide of the invention is able to specifically bind to an FGF polypeptide. Preferably, the FGFR polypeptide also has a tyrosine kinase activity that may be activated upon binding of the receptor to an FGF ligand and/or upon dimerization of the FGF receptor (*i.e.*, by the binding of a first FGFR polypeptide to a second, preferably identical, FGFR polypeptide). Activation of an FGFR polypeptide may also stimulate one or more biological activities that are associated with FGF signaling. For example, activation of an FGFR polypeptide in cells (*e.g.*, by binding an FGF ligand and/or receptor dimerization) may stimulate activities such as cell mitogenesis or angiogenesis.

FGFR polypeptides, like their ligands, are known in the art (see, in particular, the references cited, supra). In particular, at least four types of FGFR polypeptide, known individually as FGFR1-FGFR4, are believed to exist (see, e.g., Jaye et al., Biochimica et Biophysica Acta 1992, 1135:185-199). Each of these FGFR polypeptides comprises a cytoplasmic domain that typically exhibits a tyrosine kinase activity, a transmembrane helix

domain, and an extracellular domain. The extracellular domain normally recognizes and specifically binds to an FGF ligand, and may itself comprise at least three distinct immunoglobulin (Ig)-like domains referred to as D1-D3. Binding specificity for the FGF ligand typically resides in, and is therefore incurred by, the D2 and D3 domains and by the short linker polypeptide sequence between those two domains. See, Plotnikov et al., Cell 1999, 98:641-650; Plotnikov et al., Cell 2000, 101:413-424; and Stauber et al., Proc. Natl. Acad. Sci. U.S.A. 2000, 97:49-54 for a more detailed discussion.

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The amino acid sequence for an exemplary FGFR polypeptide, known as FGFR1, is shown here in FIG. 2A (SEQ ID NO:3). The FGFR1 amino acid sequence is also available from GenBank and has the Accession No. P11362 (GI:120046). In this exemplary FGFR polypeptide, the D1 domain corresponds to amino acid residues 30-119. The D2 domain corresponds to amino acid residues 149-247, whereas the D3 domain corresponds to amino acid residues 252-359. The amino acid residues connecting the D1 and D2 domains (i.e., residues 120-148) are referred to here as the D1-D2 "linker region" or the D1-D2 "linker". Similarly, amino acid residues connecting the D2 and D3 domains (i.e., residues 248-251) are referred to here as the D2-D3 "linker region" or the D2-D3 "linker". It is understood that, in preferred embodiments, the amino acid residue numbers used to delineate these separate domains are approximate.

As noted above, numerous variants (including homologs and orthologs from the same and different species of organisms) are known in the art and/or may be readily identified. Such variants, including any of the FGFR polypeptides known as FGFR1, FGFR2, FGFR3 or FGFR4, are also considered part of the present invention and may be used in the compositions and methods described herein. Such variant sequences may be identified using any of the methods described, *supra*, to identify variants (including orthologs and homologs) of an FGF polypeptide.

Thus, for example, the FGFR polypeptides of the invention also include ones encoded by nucleic acid molecules that hybridize to the complement of a nucleic acid molecule encoding another FGFR polypeptide (e.g., in a Southern hybridization experiment under defined conditions). For example, in particular embodiments, an FGF polypeptide may comprise an amino acid sequence encoded by a nucleic acid molecule that hybridizes to the complement of an FGFR1 nucleic acid sequence, such as the coding sequence set forth in

FIG. 2B (SEQ ID NO:4), under highly stringent conditions that comprise 50% formamide in 5x or 6x SSC. In other embodiments, the FGF polypeptide may comprise an amino acid sequence encoded by nucleic acid molecules that hybridize to a complement of an FGFR nucleic acid sequence (e.g., the coding sequence in FIG. 2B and SEQ ID NO:4) under moderately stringent hybridization conditions (for example, 40% formamide with 5x or 6x SSC), or under low stringency conditions (for example in 5x SSC, 0.1% SDS, 0.25% milk, no formamide, 5x SSC, or 0.5% SDS).

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In still other embodiments, FGFR polypeptides can also be identified by isolating homologous or variant FGFR gene, e.g., by PCR using degenerate oligonucleotide primes designed on the basis of a given FGFR polypeptide sequence as described below.

FGFR polypeptides of the invention also include polypeptides that comprise one or more partial or fragment FGFR amino acid sequences; *i.e.*, a portion or fragment of a full length FGFR amino acid sequence such as the full length FGFR1 sequence shown in FIG. 2A (SEQ ID NO:3). Such partial FGFR polypeptides may comprise, for example, an amino acid sequence of one or more epitopes or domains of a full length FGFR polypeptide. In one preferred embodiment, for example, a partial FGFR polypeptide comprises an amino acid sequence corresponding to at least one domain which may be, *e.g.*, an intracellular domain, a transmembrane domain, or an extracellular domain such as a D1, D2 or D3 domain. A partial FGFR polypeptide may also comprise an amino acid sequence corresponding to a combination of two or more domains from a full length FGFR polypeptide. For instance, the examples, *infra*, described the construction of an exemplary fusion polypeptide that comprises the D2 and D3 domain of the FGFR1 polypeptide sequence set forth in FIG. 2A (SEQ ID NO:3).

Partial FGFR polypeptides of the invention also include ones that comprise an amino acid sequence of one or more epitopes of a full length FGFR polypeptide. Preferably, such polypeptides contain an amino acid sequence corresponding to at least 5, at least 10, at least 15, at least 20, at least 25, or at least 50 amino acid residues of a full length FGFR polypeptide sequence (e.g., of the full length FGFR1 amino acid sequence set forth in FIG. 2A and in SEQ ID NO:3).

Truncated forms of an FGFR polypeptide can also be provided. Such truncated forms may include an FGFR polypeptide with a specific deletion of amino acid

residues. For instance, in certain embodiments amino acid residue corresponding to one or more domains of a full length FGFR polypeptide (e.g., one or more of the particular domains described, above) may be deleted from the amino acid sequence of an FGFR polypeptide.

The FGFR polypeptides of this invention include, in addition to naturally occurring homologs and orthologs of FGFR polypeptides such as FGFR1 (SEQ ID NO:3), but also include analogs and derivatives of an FGFR polypeptide. Such analogs and derivatives may be ones that are naturally occurring (such as allelic variants), or may be man made (such as fusion proteins). However, analogs and derivatives of an FGFR polypeptide will have the same or homologous characteristics of FGFR polypeptides set forth above.

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An FGFR chimeric or fusion polypeptide may also be prepared in which the FGFR portion of the fusion polypeptide has one or more characteristics of the FGFR polypeptide. Such fusion polypeptides therefore represent alternative embodiments of the FGFR polypeptides of this invention. Exemplary FGFR fusion polypeptides include ones which comprise a full length, derivative or truncated FGFR amino acid sequence, as well as fusions which comprise a fragment of an FGFR polypeptide sequence (e.g., a fragment corresponding to an epitope or to one or more domains). Such fusion polypeptides may also comprise the amino acid sequence of a second, different polypeptides; including the amino acid sequence for any of the poylpeptides described, supra, for fusion proteins of an FGF ligand.

FGFR analogs or variants can also be made by altering encoding nucleic acid molecules, including any of the alterations described, *supra*, for FGF ligand polypeptides (e.g., by substitutions, additions or deletions). Preferably, such altered nucleic acid molecules encode functionally similar molecules (i.e., molecules that perform one or more functions of an FGFR polypeptide and/or have one or more FGFR bioactivities). Thus, in a specific embodiment, an analog or variant of an FGFR polypeptide is a function-conservative analog or variant.

As with FGF ligand polypeptides, amino acid residues (other than ones that are specifically identified herein as being conserved) may differ among variants of a protein or polypeptide. Accordingly, the percentage of protein or amino acid sequence similarity between any two FGFR polypeptides may vary. The skilled artisan will recognize that the percentage of protein or amino acid sequence similarity between any two FGFR polypeptides

of similar function may vary in ways that are similar to those sequence variations described, supra, for FGF ligand polypeptides and nucleic acids.

In still other embodiments, an analog of an FGFR polypeptide may be an allelic variant or mutant FGFR polypeptide. The FGFR polypeptides of the invention also include derivative FGFR polypeptides which may be modified, e.g., according to any of the specific modifications described, supra, for FGF polypeptides.

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While the above, exemplary variants and analogs of FGFR polypeptides are described primarily in terms of the exemplary FGFR polypeptide, FGFR1, set forth in FIG. 2A (SEQ ID NO:3), it is understood that variant FGFR polypeptides of the invention include other FGFR polypeptides (e.g., naturally occurring homologs and orthologs described supra) having equivalent amino acid substitutions, deletions or insertions.

the present invention comprises a nucleic acid sequence that encodes an FGFR polypeptide (as defined, above, in this Subsection) or the complement of an FGFR polypeptide encoding sequence. The invention also provides fragments of FGFR encoding sequences and their complements, and such sequences are also considered part of the FGFR nucleic acid molecules of this invention. Thus, in one exemplary embodiment, an FGFR nucleic acid molecule of this invention may encode the exemplary FGFR1 polypeptide sequence set forth in FIG. 2A (SEQ ID NO:3), such as the particular FGFR1 nucleic acid sequence that is depicted in FIG. 2B (SEQ ID NO:4).

In still other embodiment, the FGFR nucleic acid molecules of this invention comprise nucleic acid sequences that encode one or more domains of an FGFR polypeptide; for example, an intracellular domain, a transmembrane domain, or an extracellular domain or portion thereof (e.g., a D1, D2 or D3 domain).

The FGFR nucleic acid molecules of the invention also include nucleic acids which comprise a sequence encoding one or more fragments of an FGFR polypeptide. Such fragments include, for example, polynucleotides that encode an epitope of an FGFR polypeptide; e.g., nucleic acids that encode a sequence of at least 5, and more preferably at least 10, 15, 20, 25 or 50 amino acid residues of an FGFR polypeptide sequence (for example, the exemplary FGFR1 polypeptide sequence set forth in FIG. 2B and in SEQ ID NO:4).

As explained above, numerous variant FGFR polypeptides are known in the art and/or may be readily identified by those skilled in the art, including homologous and orthologous polypeptides from the same and different species of organism. The FGFR nucleic acid molecules of the invention therefore include nucleic acid molecule comprising coding sequences for variant FGFR polypeptides (including allelic variants, analogs and homologous from the same or different species), as well as nucleic acid molecule comprising coding sequences for modified FGFR polypeptides (e.g., having amino acid substitutions, deletions or truncations). In preferred embodiments, such nucleic acid molecules have at least 50%, preferably at least 75% and more preferably at least 90% sequence identity to another FGFR coding sequence, such as the exemplary FGF2 coding sequence set forth in FIG. 2B (SEQ ID NO:4).

In addition, the FGFR nucleic acid molecules of the invention include nucleic acid molecules that hybridize to another FGFR nucleic acid molecule, e.g., in a Southern blot assay under defined conditions. For example, in specific embodiments an FGF nucleic acid molecule of the invention comprises a nucleotide sequence which hybridizes to a complement of the exemplary FGFR1 coding sequence set forth in FIG. 2B (SEQ ID NO:4) under highly stringent or moderately stringent hybridization conditions that are defined, supra, for FGF nucleic acids.. Alternatively, an FGFR nucleic acid molecule may hybridize, under the same defined hybridization conditions, to the complement of a fragment of a nucleotide sequence encoding a full length FGFR polypeptide.

In other embodiments, FGFR nucleic acid molecules of the invention comprise fragments of a full length FGFR nucleic acid sequence. Such nucleic acid fragments comprise a nucleotide sequence that corresponds to a sequence of at least 10 nucleotides, preferably at least 15 nucleotides and more preferably at least 20 nucleotides of a full length coding FGFR nucleotide sequence. In specific embodiments, the fragments correspond to a portion (e.g., of at least 10, 15, or 20 nucleotides) of the exemplary FGFR1 coding sequence shown in FIG. 2B (SEQ ID NO:4). In other embodiments, an FGFR nucleic acid fragment may comprise sequences of at least 10, preferably at least 15, and more preferably at least 20 nucleotides that are complementary and/or hybridize to a full length FGFR coding sequence (e.g., the FGFR1 coding sequence set forth in FIG. 2B and in SEQ ID NO:4) or to a fragment thereof. Suitable hybridization conditions for such oligonucleotides are described, supra, for

FGF nucleic acids.

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Nucleic acid molecules comprising such fragments are useful, for example, as oligonucleotide probes and primers (e.g., PCR primers) to detect and amplify other nucleic acid molecules encoding an FGFR polypeptide, including genes that encode variant FGFR polypeptides (including genes that encode homologous or orthologous FGFR polypeptides from the same or different species of organism). Oligonucleotide fragments of the invention may also be used, e.g., as antisense nucleic acids, triple helix forming oligonucleotides or as ribozymes (e.g., to modulate levels of FGFR gene expression or transcription in cells).

The nucleic acid molecules of the invention also include "chimeric" FGFR nucleic acid molecules. Such chimeric nucleic acid molecules are polynucleotides which comprise at least one FGFR nucleic acid sequence (which may be any of the full length or partial FGFR nucleic acid sequences described above), and also at least one non-FGFR nucleic acid sequence. For example, the non-FGFR nucleic acid sequence may be any of the non-FGF nucleic acid sequences described, *supra*. In preferred embodiments, a chimeric FGFR nucleic acid molecule of the invention encodes an FGFR fusion polypeptide of the invention.

It is understood that FGFR nucleic acid molecules of the present invention may be obtained and/or isolated using standard techniques that are known in the art and described, *supra*, for obtaining FGF nucleic acids. Similarly, FGFR polyeptides may be readily expressed, *e.g.*, by expressing FGFR nucleic acids in host cells using any of the art recognized techniques that are described above for expressing FGF polypeptides.

Agonists and Antagonists

The present invention also provides compounds that modulate FGFR activity and FGF-signaling. Such compounds are therefore useful, e.g., for modulating biological activities that are associated with FGF-signaling and/or as therapeutic agents for treating disorders associated with FGF-signaling. For example, the compounds of this invention may be used, e.g., to modulate mitogenesis, angiogenesis or differentiation of cells. Such compounds are also useful, e.g., as therpeutic agents to modulate tumor growth or to treat a disorder of cell proliferation (referred to herein as "cell proliferation disorders"), for example cancer.

Compounds that modulate FGF-signaling or an activity associated therewith may be readily identified using screening methods of the present invention. For example, the accompanying appendix provides structure coordinates, discussed in the Examples *infra*, for a dimerized ternary complex of an FGF ligand, an FGF receptor and sucrose octasulfate (SOS). Interactions (e.g., hydrogen bonding interactions) between the SOS molecule and the FGF ligand and receptor molecule(s) are also disclosed that stabilize formation of the ternary complex and, moreover, stabilize FGF receptor dimerization. Using routine, computer modeling algorithms and other techniques that are well known in the art, a user may identify other compounds that are expected to an FGF ligand and/or its receptor in a way that is similar to binding of SOS. More specifically, using the crystal structure provided here, those skilled in the art can identify compounds that bind to an FGF receptor and/or ligand, and form stabilizing interactions with the ligand/receptor complex that are similar to the stabilizing interactions described here for SOS.

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In exemplary embodiments, compounds identified by the screening methods of this invention may form a ternary complex with an FGF ligand and its receptor while, at the same time, inhibiting FGF receptor dimerization. More specifically, the compounds may be ones which have (or are expected to have) stabilizing interactions between an FGF ligand and receptor in a ternary complex that are similar to the stabilizing interactions described infra. for SOS. At the same time, however, these compounds may disrupt or inhibit stabilizing interactions between a first and second ternary complex (e.g., by eliminating key hydrogen bonding interactions) so that dimerization of the FGF receptor is inhibited. Such compounds can be expected to compete with heparin for binding to the FGF ligand and its receptor, and inhibit FGFR dimerization. Accordingly, the compounds can also be expected to inhibit FGFR activity and FGF-signaling, as well as biological activities (e.g., mitogenesis, angiogenesis, etc.) that are associated with FGF-signaling and FGFR activity. Still other compounds, such as suramin, described infra, may stabilize interactions between an FGFligand and its receptor, similar to SOS, while at the same time inhibiting FGF signaling. Such compounds are therefore referred to here as "antagonists" or as "heparin antagonists" since they suppress the action of heparin in FGF-signaling.

In other exemplary embodiments, compounds identified by screening methods of this invention may actually have (or may be expected to have) improved binding or

stabilizing interactions with an FGF ligand and/or receptor(s). For example, compounds identified by these screening methods may form (or be expected to form) stronger and/or more specific hydrogen bonding interactions with an FGF ligand or with an FGF receptor or receptors, and may actually form complexes with an increased binding affinity relative, e.g., to heparin. Such compound may also promote dimerization of an FGF receptor and thereby increasing FGFR dimerization. These compounds can be expected to increase FGFR activity and FGF-signaling, as well as biological activities that are associated with FGF-signaling and FGFR activity. Such compounds are therefore referred to here as "agonists" or "heparin agonists" since they enhance or improve upon the action of heparin in FGF-signaling.

Examples of heparin agonists and antagonists include derivatives of SOS. SOS derivatives may be determined using a rational drug design approach that utilizes the information derived from the FGF-FGFR-SOS complex crystal structure described in the Examples, *infra*. Examples of antagonists include suramin and SOS derivatives with one or more sulfate groups substituted with benzyl or trityl or other bulky hydroxyl protecting groups. Bulky groups such as these are predicted to provide a steric effect, which hampers recruitment of a second FGFR from another FGF-FGFR complex.

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SOS derivatives, which incorporate benzyl and trityl substitutions or other bulky group substitutions may be synthesized using regioselective sucrose functionalization procedures known to those skilled in the art (see, for example, Jenner & Khan, J.C.S. Chem. Comm. 1980, 50-51; Vlahov, J. Carbohydr. Chem. 1997, 16:1-10; Polat, J. Carbohydr. Chem. 1997, 16:1319-1325; and Bazin, Carbohydr. Res. 1998, 309:189-205), followed by persulfonation. Other types of hydroxyl protecting groups, such as bulky acyl groups, including but not limited to benzoyl, pivaloyl, fatty acyl groups, or bulky silyl groups such as t-butylphenylsilyl (TBDPS) or t-butylmethylsilyl (TBDMS), or bulky ketals or acetals such as isopropylidene or benzylidene, might also be used in place of the bulky benzyl and trityl ether groups.

Preferred SOS derivatives include 2-O-Bn sucrose heptasulfate (Structure I), 1'-O-Bn sucrose heptasulfate (Structure II), 1',2-di-O-Bn sucrose hexasulfate (Structure III). The exemplary synthesis of Structures I and II is illustrated in FIG. 8. The exemplary synthesis of Structure III is illustrated in FIG. 9. Specifically, structures I and II may be formed by the selective benzylation of sucrose in the 1' - or 2- positions, followed by

separation and persulfonation. Structure III may be formed using a regioselective 1',2-silylation (Jenner & Khan, *supra*) followed by peracetylation and separation. The 1',2-silyl derivative formed is desialated, the free hydroxy groups are benzylated, and the compound formed is deacetylated and persulfonated.

Still other examplary SOS derivatives include 6-O-hexadecanoyl sucrose heptasulfate (Structure V) and 2-)-dodecanoyl, 6'-O-hexadecanoyl sucrose hexasulfate (Structure VI), both of which are illustrated in FIG. 10.

Compounds identified by molecular modeling and/or the screening methods described here may be further investigated to better characterize their ability to form ternary complexes with FGF ligands and receptor, as well as for their ability to modulate FGFR dimerization and FGF-signaling. For example, a test compound may be contacted, in a reaction mixture, to an FGF ligand, and to an FGF receptor in either the presence or, alternatively, in the absence of co-factors such as heparin. The reaction mixture can then be assayed to determine whether a ternary complex has formed using techniques, such as size exclusion chromatography (see the Examples, *infra*), that are well known in the art. In preferred embodiments, such assays may also determine whether such ternary complexes have dimerized to indicate whether FGFR dimerization has been enhanced or inhibited by the test compound.

In vivo or cell culture assays may also be used to determine whether a test compound functions as a heparin agonist or antagonist to modulate FGFR activity or FGF-signaling in cells. For instance, the Examples, infra, describe cell culture assays that may be used to measure a test compound's ability to modulate an activity, such as mitogenesis, that is associated with FGF-signaling. Such assays generally comprise contacting a test compound to a cell that expresses an FGF receptor. The test compound should be contacted to the cell in the presence of an FGF ligand and, optionally, in the presence of a co-factor such as heparin or HSPG that activates FGFR. The cell culture may then be assayed or examined to determine whether a response associated with FGF-signaling has been activated. For instance, the Examples infra provide an assay that test the ability of a test compound to modulate cell growth (i.e., mitogenesis) stimulated by FGF-signaling.

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Pharmaceutical Preparations. In preferred embodiments, compounds that are

agonists or antagonists of FGFR activity and/or of FGF-signaling may be administered (e.g., in vitro or ex vivo to cell cultures, or in vivo to an organism) at therapeutically effective doses to treat a disease or disorder associated with FGF-signaling. Such compounds may be used, for example, to modulate activities such a mitogenesis and angiogenesis, or to modulate (preferably decrease) tumor growth. Exemplary diseases that may be treated using such methods include cell proliferative disorders such as cancer. Accordingly, the invention also provides pharmaceutical preparations for use, e.g., as therapeutic compounds for the treatment of disorders and other conditions that are associated with FGF-signaling and/or FGFR activity.

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The terms "therapeutically effective dose" and "effective amount" refer to the amount of the compound that is sufficient to result in a therapeutic response. In embodiments where a compound (e.g., a drug or toxin) is administered in a complex (e.g., with an FGF or FGFR specific antibody), the terms "therapeutically effective dose" and "effective amount" may refer to the amount of the complex that is sufficient to result in a therapeutic response. A therapeutic response may be any response that a user (e.g., a clinician) will recognize as an effective response to the therapy. Thus, a therapeutic response will generally be an amelioration of one or more symptoms of a disease or disorder. In preferred embodiments, where the pharmaceutical preparations are used to treat a cancer, a therapeutic response may be a reduction in the number of cancer cells observed, e.g., in biopsies from a patient during treatment. Alternatively, an effective therapeutic response may be a reduction or shrinkage in the size of one or more tumors.

Toxicity and therapeutic efficacy of compounds can be determined by standard pharmaceutical procedures, for example in cell culture assays or using experimental animals to determine the LD₅₀ and the ED₅₀. The parameters LD₅₀ and ED₅₀ are well known in the art, and refer to the doses of a compound that are lethal to 50% of a population and therapeutically effective in 50% of a population, respectively. The dose ratio between toxic and therapeutic effects is referred to as the therapeutic index and may be expressed as the ratio: LD₅₀/ED₅₀. Compounds that exhibit large therapeutic indices are preferred. While compounds that exhibit toxic side effects may be used. However, in such instances it is particularly preferable to use delivery systems that specifically target such compounds to the site of affected tissue so as to minimize potential damage to other cells, tissues or organs and

to reduce side effects.

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Data obtained from cell culture assay or animal studies may be used to formulate a range of dosages for use in humans. The dosage of compounds used in therapeutic methods of the present invention preferably lie within a range of circulating concentrations that includes the ED_{50} concentration but with little or no toxicity (e.g., below the LD_{50} concentration). The particular dosage used in any application may vary within this range, depending upon factors such as the particular dosage form employed, the route of administration utilized, the conditions of the individual (e.g., patient), and so forth.

A therapeutically effective dose may be initially estimated from cell culture assays and formulated in animal models to achieve a circulating concentration range that includes the IC₅₀. The IC₅₀ concentration of a compound is the concentration that achieves a half-maximal inhibition of FGF signaling activity (e.g., as determined from the cell culture assays) or, where a compound is administered to treat a particular disorder, a half-maximal inhibition of symptoms. Appropriate dosages for use in a particular individual, for example in human patients, may then be more accurately determined using such information.

Measures of compounds in plasma may be routinely measured in an individual such as a patient by techniques such as high performance liquid chromatography (HPLC) or gas chromatography.

Pharmaceutical compositions for use in accordance with the present invention may be formulated in conventional manner using one or more physiologically acceptable carriers or excipients.

Thus, the compounds and their physiologically acceptable salts and solvates may be formulated for administration by inhalation or insufflation (either through the mouth or the nose) or oral, buccal, parenteral or rectal administration.

For oral administration, the pharmaceutical compositions may take the form of, for example, tablets or capsules prepared by conventional means with pharmaceutically acceptable excipients such as binding agents (e.g., pregelatinised maize starch, polyvinylpyrrolidone or hydroxypropyl methylcellulose); fillers (e.g., lactose, microcrystalline cellulose or calcium hydrogen phosphate); lubricants (e.g., magnesium stearate, talc or silica); disintegrants (e.g., potato starch or sodium starch glycolate); or wetting agents (e.g., sodium lauryl sulphate). The tablets may be coated by methods well known in the art. Liquid

preparations for oral administration may take the form of, for example, solutions, syrups or suspensions, or they may be presented as a dry product for constitution with water or other suitable vehicle before use. Such liquid preparations may be prepared by conventional means with pharmaceutically acceptable additives such as suspending agents (e.g., sorbitol syrup, cellulose derivatives or hydrogenated edible fats); emulsifying agents (e.g., lecithin or acacia); non-aqueous vehicles (e.g., almond oil, oily esters, ethyl alcohol or fractionated vegetable oils); and preservatives (e.g., methyl or propyl-p-hydroxybenzoates or sorbic acid). The preparations may also contain buffer salts, flavoring, coloring and sweetening agents as appropriate.

Preparations for oral administration may be suitably formulated to give controlled release of the active compound. For buccal administration the compositions may take the form of tablets or lozenges formulated in conventional manner. For administration by inhalation, the compounds for use according to the present invention are conveniently delivered in the form of an aerosol spray presentation from pressurized packs or a nebuliser, with the use of a suitable propellant, e.g., dichlorodifluoromethane, trichlorofluoromethane, dichlorotetrafluoroethane, carbon dioxide or other suitable gas. In the case of a pressurized aerosol the dosage unit may be determined by providing a valve to deliver a metered arrount. Capsules and cartridges of e.g., gelatin for use in an inhaler or insufflator may be formulated containing a powder mix of the compound and a suitable powder base such as lactose or starch.

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The compounds may be formulated for parenteral administration by injection, e.g., by bolus injection or continuous infusion. Formulations for injection may be presented in unit dosage form, e.g., in ampules or in multi-dose containers, with an added preservative. The compositions may take such forms as suspensions, solutions or emulsions in oily or aqueous vehicles, and may contain formulatory agents such as suspending, stabilizing and/or dispersing agents. Alternatively, the active ingredient may be in powder form for constitution with a suitable vehicle, e.g., sterile pyrogen-free water, before use.

The compounds may also be formulated in rectal compositions such as suppositories or retention enemas, e.g., containing conventional suppository bases such as cocoa butter or other glycerides.

In addition to the formulations described previously, the compounds may

also be formulated as a depot preparation. Such long acting formulations may be administered by implantation (for example subcutaneously or intramuscularly) or by intramuscular injection. Thus, for example, the compounds may be formulated with suitable polymeric or hydrophobic materials (for example as an emulsion in an acceptable oil) or ion exchange resins, or as sparingly soluble derivatives, for example, as a sparingly soluble salt.

The compositions may, if desired, be presented in a pack or dispenser device that may contain one or more unit dosage forms containing the active ingredient. The pack may for example comprise metal or plastic foil, such as a blister pack. The pack or dispenser device may be accompanied by instructions for administration.

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EXAMPLES

The present invention is also described by means of particular examples. However, the use of such examples anywhere in the specification is illustrative only and in no way limits the scope and meaning of the invention or of any exemplified term. Likewise, the invention is not limited to any particular preferred embodiments described herein. Indeed, many modifications and variations of the invention will be apparent to those skilled in the art upon reading this specification and can be made without departing from its spirit and scope. The invention is therefore to be limited only by the terms of the appended claims along with the full scope of equivalents to which the claims are entitled.

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Example 1: SOS Promotes Dimerization of FGF - FGFR Complexes

This example describes experiments that were performed *in vitro* to test whether sucrose octasulfate (SOS) can act as a heparin mimetic. Specifically, the data obtained from these experiments demonstrate that SOS is able to promote the dimerization of complexes between fibroblast growth factor receptors and their ligands (*i.e.*, FGF - FGFR complexes).

A construct encoding an extracellular ligand binding portion of the FGFR1 polypeptide set forth in FIG. 1A (SEQ ID NO:1) was expressed in *E. coli* and refolded *in vivo* using established protocols, as previously described by Plotnikov *et al.* (*Cell* 2000, 101:413-424). In particular, the soluble FGFR1 polypeptide expressed by this construct, which is referred to here as D23, comprises amino acid residues 142 to 365 of SEQ ID NO:1,

which correspond to the immunoglobulin (Ig)-like domains 2 and 3 (D2 and D3, respectively), which are known to confer ligand binding and specificity for the FGFR receptor. However, the D23 polypeptide is missing the Ig-like domain 1 (D1), the acid box and the linker polypeptide sequence between D3 and the transmembrane helix. The D23 polypeptide is therefore similar to a naturally occurring splice variant of FGFR1 that retains full ligand binding capacity (Johnson et al., Mol. Cell. Biol. 1990, 10:4728-4736).

When expressed in *E. coli* cells, the D23 polypeptide was found entirely in inclusion bodies. The polypeptide was solubilized using standard denaturing reagents and refolded *in vitro*. Following purification by ion exchange chromatography, the D23 polypeptide was complexed with the FGF2 ligand polypeptide whose amino acid sequence is set forth in FIG. 2A (SEQ ID NO:3) and purified by size exclusion chromatography.

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To quantitate dimerization, the purified 1:1 FGF2:FGFR1 complexes were mixed at various molar ratios with SOS and analyzed by size exclusion chromatography according on SUPERDEX 200 ® (Amersham Pharmacia Biotech.) size exclusion column in 25 mM HEPES-NaOH buffer (pH 7.5) containing 150 mM sodium chloride. The resulting chromatograms are shown in FIGS. 3A-C.

In the absence of SOS (FIG. 3A) only a peak corresponding to monomers of the FGF:FGFR complexes are observed, which is indicated by the letter M. A small peak, identified in FIG. 3A by the letter L, was also observed at higher elution volumes. This peak corresponds to free FGF ligand polypeptide that dissociates from the FGF:FGFR complex due to protein dilution during the chromatography process. As SOS is added to the mixture (FIGS. 3B-3C), a third peak corresponding to dimers of the FGF:FGFR complex is observed (identified by the letter D) while the intensity of the monomer peak (M) decreases. The intensities of the dimer and monomer peaks increase and decrease, respectfully, as SOS is added in higher amounts (compare, e.g., FIG. 3B to FIG. 3C). Finally, when SOS is added at a 1:1:1 molar ratio to the FGF and FGFR (FIG. 3D), only a peak corresponding to FGF:FGFR dimers is observed.

Similar results have also been obtained by the inventors in size exclusion chromatography experiments that used a homogenously sulfated heparin hexasacharide instead of a SOS (see, in particular, Schlessinger et al., Molecular Cell 2000, 6:743-750). However, the results presented here show that small molecules, including sulfated discharides

such as SOS, can dimerize an FGF receptor.

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Example 2: SOS Promotes Activation of the FGF Receptor by FGF in Cells

This example describes experiments that investigated the ability of SOS to modulate FGF ligand-dependent activation of the FGF receptor *in vivo*. In particular, an assay is described here that uses a BaF3 cell line which overexpresses FGFR1. This cell line has been previously described and is therefore known in the art (see, e.g., Huang et al., J. Biol. Chem. 1995, 270:5065-5072).

BaF3 cells are a lymphoid cell line, which are dependent on interleukin-3 (IL-3) for growth. Ordinarily, these cells do not exhibit any response to FGF. However, when stably transfected to express an FGF receptor, the cells exhibit a dose-dependent mitogenic response to FGF ligand in the absence of IL-3. Accordingly, the growth rate of such transfected cells is useful as a measurement of FGF receptor activity *in vivo*. Because BaF3 cells express only low amounts of HSPG, soluble heparin must also be present to elicit the FGF-dependent mitogenic response observed in the transfected cells.

For the experiments discussed here, BaF3 cells that stably expressed wild-type FGFR1 (SEQ ID NO:1) were cultured according to standard methods that have been previously described (see, Huang *et al.*, *supra*). 1×10^4 cells were seeded in triplicate wells and grown in the presence of heparin (3 μ M) or, alternatively, in the presence of various concentrations (0.1, 0.5, 1, 5 and 10 μ M, respectively) of SOS. The numbers of viable cells in each well were counted daily in duplicate.

Data from these experiments are graphically presented here in **FIG. 4** as mean and standard deviation values. As can be seen from inspecting the figure, SOS supports FGF2 in inducing proliferation of the BaF3 cells over expressing FGFR1 in a dose-dependent manner. As anticipated, the BaF3 cells grow minimally in the presence of FGF2 alone.

Thus, these data complement data from the *in vitro* experiments presented in Example 1, *supra*. In particular, these experiments demonstrate not only that SOS can bind to and/or support dimerization of FGF ligand-receptor complexes, but also show that SOS can increase FGF receptor activity in cells, and thereby enhance signaling by an FGF ligand.

Example 3: Crystallography of an FGF-FGFR Complex with SOS

This example describes x-ray crystallography experiments that better characterize the molecular mechanisms by which SOS may interact with and/or stabilize dimers of FGF-FGFR complexes. In particular, this example describes the crystalization of FGF2-FGFR1 complexes with SOS and the solution of that crystal structure by analyzing x-ray diffraction data.

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Crystals of dimeric FGF2-FGFR1-SOS complexes were grown by vapor diffusion at 20 °C using the hanging drop method. 2 μL of protein solution (10 mg/mL in 25 mM HEPES-NaOH (pH 7.5) and 150 mM NaCl) was mixed with an equal volume of crystallization buffer (12-16% Polyethylene glycol 5000, 0.2 M ammonium sulfate and 15% glycerol in 0.1 M HEPES-NaOH (pH 7.5)). The protein solution contained a 1:1:1 stoichiometric ratio of FGF2, and soluble FGFR1 construct described, *supra*, in Example 1, and SOS.

The resultant crystals are shown in FIG. 5A. The crystal belongs to the orthorhombic space group P2₁ 2₁ 2₁ and has unit cell dimensions of a = 64.2 Å, b = 122.4 Å and c = 219.5 Å. The crystal contains four FGF2-FGFR1-SOS complexes in the asymmetric unit with a solvent content of about 56%.

Diffraction data were collected from a flash-frozen crystal on a CCD detector at beamline X4A at the National Synchrotron Light Source, Brookhaven National Laboratory. The data were processed using DENZO and SCALEPACK (Otwinowski & Minor, *Methods Enzymol.* 1997, 276:307-326). A molecular replacement solution was found for the four copies of the ternary FGF2-FGFR1-SOS complex in the asymmetric unit using the program AmoRe (Navaza, *Acata. Crystallogr. Sect. A* 1994, 50:157-163) and the binary FGF2-FGFR1 crystal structure deposited in the Protein Data Bank (see, Berman *et al.*, *Nucl. Acids Res.* 2000, 28:235-242) under ID code 1CVS (Plotnikov, *Cell* 1999, 98:641-650) as the search model.

The initial model for the structure of SOS was taken from the FGF1-SOS crystal structure deposited in the Protein Data Bank under ID code 1AFC (Zhu et al., Structure 1993, 1:27-34). Parameters for the SOS molecule were generated using the HIC-Up server (Kleywegt & Jones, Acta. Crystallogr. D 1998, 54:1119-1131). The models were refined by simulated annealing and positional/B-factor refinement using CNS (Brunger et al., Acta Crystallogr. Sect. D 1998, 54:905-921) with bulk solvent and anisotropic B-factor

corrections applied. Tight noncrystallographic symmetry restrains were imposed throughout the refinement for the backbone atoms of FGF2 domains D2 and D3. Model building into the $2F_0$ - F_0 and F_0 - F_0 electron density maps was performed with the program O (Jones *et al.*, *Acta Crystallogr. Sect. A* 1991, 47:110-119).

From these methods, the crystal structure has been refined to a 2.6 Å resolution with an R value of 24% (free R value of 28%). The atomic model consists of four FGF2 molecules (residues 16 to 144 from SEQ ID NO:1), four FGFR2 molecules (residues 149 to 359 from SEQ ID NO:3), four SOS molecule, three sulfate ions and 42 molecules of water. A list of coordinates for the final structure is provided here, in PDB file format, at the Appendix *infra*. Data collection and refinement statistics are given in Table 1, below.

TABLE 1: Summary of crystallographic analysis

Resolution (Å)	Reflections (total/uniqu		eness (%)	R _{sym} * (%)	Signal (⟨⟨σ·¹≻)
30.0-2.6	764014/53	698 99.9 (100	00.0) ^b 7.8 (33	7.8 (33.2) ^b	13.5
1. Refinement	Statistics:c				
-	•	•	Root-mean-square Deviations		
Resolution (Å)	Reflections	R _{cryst} /R _{free} d (%)	Bonds (Å)	Angles (°)	B-factors (Å
25.0-2.6	52014	24.1/27.8	0.008	1.4	1.00

20 • $R_{om} = 100 \times \sum_{ij} \sum_{l} |l_{i}(hkl) - \langle l(hkl) \rangle | / \sum_{ij} \sum_{l} |l_{i}(hkl)|$.

^o Atomic model: 10823 protein atoms, 4 SOS molecules, 3 SO₄² ions and 42 water molecules.

 ${}^{d}R_{crysilfree} = 100 \times \sum_{hkl} ||F_o(hkl)| - |F_c(hkl)|| / \sum_{hkl} |F_o(hkl)||$, where F_o (>0 σ) and F_c are the observed and calculated structure factors. 5% of the reflections were used for calculations of R^{free} .

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EXAMPLE 4: Analysis of the Dimerized FGF-FGFR-SOS Crystal Structure

Coordinates for the final refined crystal structure of the FGF-FGFR dimer complex with SOS is provided here, in PDB format, in the accompanying Appendix.

b Value in parentheses is for the highest resolution shell: 2.69 - 2.6 Å.

^{*} For bonded protein atoms.

Description of the overall structure. The four 1:1:1 FGF2-FGFR1:SOS complexes of the crystals' asymmetric unit are arranged into two dimeric assemblies. Each dimer structure closely resembles the dimeric assembly of the binary FGF2-FGFR1 complexes describes previously by Plotnikov et al. (Cell 1999, 98:641-650), and may be viewed conceptually as the association of two 1:1:1 ternary complexes of FGF2:FGFR2:SOS. The structure of the FGF2:FGFR2:SOS dimers was visualized using the Molscript and Raster3D programs (see, Kraulis, J. Appl. Crystallogr. 1991, 24:946-950; and Merritt & Bacon, Methods Enzymol. 1997, 277:505-524). The overall structure for one dimer complex is illustrated in FIG. 5B. The same structure is also illustrated in FIG. 5C, as viewed when the structure illustrated in FIG. 5B is rotated 90° around the horizontal axis. The F_o-F_c electron density map computed after simulated annealing with SOS omitted from the atomic model was also visualized using the Bobscript program (see, Esnouf, J. Mol. Graph. Model 1997, 15:132-134), and is shown in FIGS. 6A-B.

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Within each ternary complex, the FGF2 ligand binds to the D2 and D3 domains of the receptor FGFR1, as well as to the linker sequence between the D2 and D3 domains of FGFR1. The dimer, in turn, is held together by interactions of the FGF2, FGFR1 and SOS from one ternary complex with the FGFR1 in the other, adjoining ternary complex within the dimer.

The SOS binding site. Each dimer in the crystals' asymmetric unit contains two SOS molecules, which bind to the same general region of the FGF-FGFR1 dimer complex that has been shown to bind heparin (see, Schlessinger et al., Molecular Cell 2000, 6:743-750). As can be seen in FIG. 6, the F_o-F_c electron density for one of the SOS molecules is strong and well contoured, while the density for the second SOS molecule is less defined, indicating that this second SOS molecule is somewhat less ordered within the crystals. The well ordered SOS molecule makes a total of 13 hydrogen bonds with on FGF2 and both FGFR1 molecules in the asymmetric unit. These H-bonds, which are illustrated in FIG. 7, stabilize the FGF2-FGFR1 complexes, and also promote dimerization.

Interactions of SOS with FGF and FGFR in the dimer. Within each ternary complex, SOS makes five hydrogen bonds with FGF2 and four with FGFR1. These hydrogen

bonding interactions are illustrated schematically in FIG. 7. Specifically, hydrogen bonding interactions are observed between both the 5- and 6- membered rings of SOS and Lysines 163 and 177 of FGFR1. These lysines are located on the heparin binding surface of the D2 domain in FGFR1, and have also been shown to bind heparin in the crystal structure of a FGF2-FGFR1 complex with heparin (see, Schlessinger et al., Molecular Cell 2000, 6:743-750).

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SOS also interacts with the D2 domain of the FGFR molecule in the adjoining ternary complex of the crystals' asymmetric unit. Specifically, a hydrogen bond is observed between Lysine 207 of the second FGFR molecule and the 2-sulfate (in the 6-membered ring) of SOS. Another hydrogen bond is observed between Lysine 207 of the second FGFR molecule and the 6'-sulfate (in the 5-membered ring) of SOS. Interestingly, Lysine 207 has also been implicated in heparin binding (see, Schlessinger *et al.*, *supra*). Two addition hydrogen bonds, mediated by a water molecule, are observed between the 6'-sulfate of SOS and backbone atoms in the glycine 205 and aspartic acid 218 amino acid residues of the second FGFR molecule.

Five additional hydrogen bonds are made between Lysines 26 and 135 of FGF2 and the sulfate groups of SOS. In the crystal structure of a ternary FGF2-FGFR1-heparin complex described by Schlessinger *et al.*, *supra*, these FGF2 lysines form hydrogen bonds to heparin.

Thus, the crystal structure described here demonstrates that SOS interacts with FGF and FGFR in a way that mimics the proteins' reaction with heparin, and similarly increases FGF-FGFR binding affinity.

EXAMPLE 5: Heparin Agonists and Antagonists as Therapeutic Agents

The experiments described in Examples 1-4, *supra*, demonstrate that SOS can interact with an FGF ligand and/or its receptor and, moreover, that this interaction enhances dimerization of the receptor-ligand complex, and increases receptor activity. Recent biochemical and structural data have indicated that FGF may form an initial, low affinity complex with FGFR in the absence of heparin (see, *e.g.*, Pantoliano *et al.*, *Biochemistry* 1994, 33:10229-10248; and Plotnikov *et al.*, *Cell* 1999, 98:641-650). However, this minimal 1:1 complex may, at best, only allow transient receptor dimerization and signaling at high, non-

physiological concentrations of the receptor and/or its ligand. Under normal physiological concentrations, the FGF ligand and its receptor tend to dissociate, and do not have sufficient oportunity to interact simultaneously with a second FGF receptor. Without being bound to any particular theory or mechanism of action, it is therefore believed that the presence of either heparin or SOS is necessary under normal physiological concentrations of FGF ligand and/or receptor to stabilize the low affinity receptor-ligand complexes, and provide sufficient opportunity for the concerted binding of FGF ligand and receptor in one monomeric ternary complex to the FGFR in a second monomeric ternary complex. In other words, both heparin and SOS are believed to bind to FGF ligand and receptor and generate stable receptor-ligand complexes which, in turn, provide sufficient interface for the binding of a second FGF receptor molecule.

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The crystal structures described in Example 4, supra; provide, for the first time, specific interactions that stabilize an FGF ligand-receptor complex and, moreover, additional interactions between SOS and a second FGF receptor which stabilize dimerization. The results presented in these example therefore provide an excellent framework for the development of novel therapeutic agents. The discovery is particularly useful in view of the current limitations in large-scale preparation of homogenous heparin oligosaccharides for therapeutic purposes (see, Pervin et al., 1995). In contrast, total de novo synthesis of homogenously sulfated sucrose derivatives is straightforward and known in the art. See, for example, Vlahov et al., J. Carbohydr. Chem. 1997, 16:1-10; Polat et al., J. Carbohydr. Chem. 1997, 16:1319-1325; and Bazin et al., Carbohydr. Res. 1998, 309:189-205. Exemplary, non-limiting examples of such therapeutic compounds are described here, along with some particular examples of their utility as therapeutic agents.

Heparin antagonists. Compounds that may be used as therapeutic agents of the present invention include ones that function or are likely to function as heparin antagonist by competing with heparin to sequester FGF-FGFR complexes in a "signaling-incompetent" state. In particular, preferred therapeutic compounds of the invention include suramin and derivatives of sucrose octasulfate (SOS) that retain SOS's ability to generate stable FGF-FGFR complexes while, at the same time, inhibiting dimerization or signaling ability of those complexes. Example 5, described supra, demonstrates that suramin can interact with a pre-

formed FGF ligand-receptor complex, thereby stabilizing the interaction, while inhibiting signaling through the FGF receptor. Other exemplary heparin antagonists of the invention include derivatives of compounds such as inositol hexasulfate and sulfated β -cyclodextrin, as well as derivatives of other compounds that behave in an analogous manner to SOS and promote signaling competent dimers of the FGF ligand and receptor. As with heparin antagonists that are derivatives of SOS, heparin antagonists that are derivatives of some other compound (e.g., inositol hexasulfate or sulfated β -cyclodextrin) have the ability to generate stable FGF-FGFR complexes while, at the same time, inhibiting dimerization of those complexes. Thus, preferred heparin antagonists are compounds that generate stable, dimerization incompetent complexes of FGF-FGFR.

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In one preferred embodiment, heparin antagonists of the invention include SOS derivatives having one or more substitutions of sulfates that are involved in stabilizing interactions between a first FGF-FGFR complex and a second FGF receptor. Specific examples of such substitutions, that are particularly preferred, including substitutions at either the 2- and/or the 1' positions of SOS. Preferred substitutions include, but are not limited to, substitutions of a bulky group such as a benzyl, benzoyl, pivaloyl, fatty acyl, trityl or isopropylidene moiety for one or more sulfate moieties. However, any moiety that may be reasonably expected to block or inhibit hydrogen bonding interactions between SOS and FGFR which stabilize dimerization may be used as a substituent.

In another preferred embodiment, the heparin antagonist of the invention is suramin, a polysulfonated napthylurea that induces dimerization of pre-formed binary FGF2-FGFR1 complexes that are signaling incompetent. Without being limited to a particular mechanism or theory, the non-productive dimers may be a result of nonproductive spatial positioning of the FGFR D3 regions in the dimeric assemblies. However, the preliminary data presented in Example 5, *supra*, cannot exclude other potential models.

In yet another preferred embodiment, heparin antagonists of the invention include sulfated derivatives of a cyclodextrin compound such as sulfated derivatives of acyclodextrin, β -cyclodextrin and γ -cyclodextrin. Cyclodextrin compounds are known in the art (see, for example, Hileman *et al.*, *Electrophoresis* 1998, 19(15):2677-2681). The compounds are generally defined as a cyclic ring of $1 \rightarrow 4$ linked glucose residues. A general structural formula for derivatives of a preferred cyclodextrin, β -cyclodextrin, is provided in

FIG. 14 (Structure VIII).

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Cyclodextrin compounds are typically classified based on the number of 1-4 linked glucose residues present in the ring, with rings of between 6 and 12 glucose residues being preferred. Rings of 6, 7 and 8 glucose residues are particularly preferred. Thus, cyclodextrin compounds that comprise a ring of six 1-4 linked glucose residues (i.e., n=6) are referred to as α -cyclodextrin compounds. Cyclodextrin compounds that comprise a ring of seven 1-4 linked glucose residues are referred to as β -cyclodextrin compounds (FIG. 14, Structure VIII) and cyclodextrin compounds that comprise a ring of eight 1-4 linked glucose residues are referred to as γ -cyclodextrin compounds. Referring to the general structure provided in FIG. 14 (Structure VIII), each of the group labeled "R" on each of the glucose residues is generally a hydrogen. However, other chemical moieties may be substituted for these groups to form cyclodextrin derivative compounds; such as sulfated cyclodextrin or sulfonated cyclodextrins.

Preferred cyclodextrin compounds that are heparin antagonists are sulfated cyclodextrin. Each group R on each of the glucose residues in a sulfated cyclodextrin preferably is independently a hydrogen (H) or a sulfate group (SH). At least one sulfate group must be present. However, it is more preferably that at least about 50% or more (e.g., at least 60%, 70%, 80%, 90%, 95%, 99% or 100%) of the cyclodextrin hydroxyl residues is sulfated. Generally, a sulfated cyclodextrin molecule used in the methods and compositions of the present invention may comprise a mixture of sulfated cyclodextrin molecules, with each molecule preferably comprising the same number of glucose residues in the cyclodextrin ring but having different hydroxyl residues and/or different numbers of hydroxyl residues substituted with a sulfate group.

Heparin antagonists, such as the ones described hereabove, are expected to inhibit dimerization or signaling of an FGF receptor and therefore decrease FGFR mediated signaling. Such compounds may be useful, therefore, as agents for inhibiting biological activities associated with FGFR signaling or activity including, for example, angiogenesis and tumor growth.

FIGS. 8-11 illustrate the exemplary synthesis of six other preferred SOS derivatives (structures I, II III, IV, V and VI) that may be used as heparin antagonists in the present invention. For example, in one preferred embodiment the SOS derivative may be 2-

O-Bn sucrose heptasulfate (structure I). In another preferred embodiment an SOS derivative may be 1'-O-Bn sucrose heptasulfate (structure II). In yet another preferred embodiment, an SOS derivative of the invention may be 1',2-di-O-Bn sucrose hexasulfate (structure III). Other preferred, exemplary SOS derivatives of the invention may include 4,6-O-isopropyliden sucrose hexasulfate (Structure IV), 6'-O-hexadecanoyl sucrose heptasulfate (Structure V) and 2-)-dodecanoyl, 6'-O-hexadecanoyl sucrose hexasulfate. Still other compounds, including other SOS derivatives, which may be used in the methods of this invention will be readily apparent to those skilled in the art given what is taught in this specification. Such compounds may also be readily synthesized by chemical reactions such as the ones illustrated in FIGS. 8 through 11 that are routine and well known in the art (see, for example, Pervin et al., Glycobiology 1995, 5:83-95; Desai et al., Carbohydr. Res. 1995, 275:391-401; Vlahov et al., J. Carbohydr. Chem. 1997, 16:1-10; Polat et al., J. Carbohydr. Chem. 1997, 16:1319-1325; Bazin et al., Carbohydr. Res. 1998, 309:189-205; Jenner & Khan, J.C.S. Chem. Comm. 1980, pp. 50-51).

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Heparin agonists. Compounds that may be used in the methods of this invention further include ones that function or are likely to function as heparin agonists. In particular, the compounds of the present invention include derivatives of sucrose octasulfate (SOS) and other compounds that enhance or promote the dimerization of FGF receptor-ligand complexes. Other exemplary heparin agonists of the invention include compounds such as inositol hexasulfate, sulfonated β -cyclodextrin, and derivatives thereof that enhance or promote the dimerization of FGF receptor-ligand complexes.

Generally, such compounds can be identified by those skilled in the art as having stabilizing interactions (for instance, hydrogen bonding interactions) in an FGF-FGFR dimer structure that preserve the stabilizing interactions observed in the FGF-FGFR dimer structure described in the above Examples. Indeed, those skilled in the art will appreciate that compounds which may be used as heparin agonists in the present invention may even have stabilizing interactions that are stronger than, or at least similar to, those in the FGF-FGFR-SOS ternary complex structures described here.

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The examples, *supra*, demonstrate that compounds such as SOS and derivatives thereof may effectively function as heparin agonists, and effectively increase cell

signaling activities mediated by an FGF ligand and/or its receptor. Thus, such compounds are useful for increasing activities that are associated with FGF signaling including, for example, tyrosine kinase activity and angiogenesis. Such compounds are particularly useful in applications where it is desirable to promote a biological activity stimulated by FGF signaling. For example, in one preferred embodiment a heparin agonist may be used to promote wound healing in an individual, e.g., by promoting mitogenic activity. In other preferred embodiments, heparin agonists of the invention (for example, sulfated inositols and sulfated β -cyclodextrins) may be used to treat disorders such as stomach ulcers by promoting dimerization of an FGF receptor-ligand complex.

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In particularly preferred embodiments, heparin agonists of the invention include sulfonated derivatives of a cyclodextrin compound, including sulfonated derivatives of α -cyclodextrin, β -cyclodextrin and γ -cyclodextrin. For instance, Example 7, *infra*, describes experiments demonstrating that sulfonated β -cyclodextrin is an effective heparin agonist.

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Cyclodextrin compounds are described, *supra*, in connection with preferred heparin antagonists of this invention and a general structural formula for a derivatives of a preferred cyclodextrin, β-cyclodextrin, is provided in FIG. 14 (Structure VIII). Preferred cyclodextrin compounds that are heparin agonists are sulfonated cyclodextrins. Each group R on each of the glucose residues of a sulfonated cyclodextrin preferably is independently a hydrogen (H) or a sulfonate group (SO₃), although other substituents may also be present. At least one sulfonate group must be present. However, it is more preferable that at least about 50% or more (*e.g.*, at least 60%, 70%, 80%, 90%, 95% or 100%) of the cyclodextrin hydroxyl residues is sulfonated. Generally the sulfonated cyclodextrin molecules used in the methods and compositions of the present invention may comprise a mixture of sulfonated cyclodextrin molecules, with each molecule preferably comprising the same number of glucose residues in the cyclodextrin ring but having different hydroxyl residues and/or different numbers of hydroxyl residues substituted with a sulfonate group.

EXAMPLE 6: Suramin Promotes Formation of FGFR Dimers That Are Signal Incompetent

This example describes experiments that investigate the ability of another compound, suramin, to modulate FGF ligand-dependent activation of an FGF receptor.

Specifically, the data presented in this example demonstrates that suramin can interact with FGF receptor-ligand complexes, and promotes dimerization of the FGF receptor. Unlike SOS, however, the FGFR dimers formed with suramin are actually signaling incompetent. Thus, these examples demonstrate an alternative mechanism by which certain compounds, including suramin, may act as agonists or FGF-mediated signaling.

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Suramin is a polysulfonated napthylurea with has the chemical structure set forth in FIG. 12 (Structure VII). The compound has demonstrated anti-tumor activity against a variety of different types of cancers, including breast cancer, prostate cancer, sarcoma, colorectal cancer, Karposi's sarcoma, non-Hodgikin's lymphoma, renal cell carcinoma and adrenal carcinoma to name a few. See, for example, Voogd et al., 1993; La Rocca et al.). The compound's anti-tumor activity may be due to an ability to bind to and inhibit FGF (see, Takano et al., 1994; Waltenberger et al., 1996). Indeed, suramin has been demonstrated to bind an FGF1 ligand and induce its aggregation (Middaugh et al., 1992). At present, however, no structural data are available to indicate how suramin might interact with an FGF ligand or receptor.

In these experiments, two milligram aliquots of the purified FGF2-FGFR1 complex described, *supra*, in Example 1 were mixed with suramin and analyzed on a size exclusion column equilibrated with 25 mM HEPES-NaOH buffer (pH 7.5) containing 150 mM NaCl. The resulting chromatograms are shown in FIGS. 13A-13D.

In the absence of suramin (FIG. 13A), only a peak corresponding to monomers of the FGF:FGFR complex are observed, which is indicated by the letter M. A small peak, identified in FIG. 13A by the letter L, was also observed at higher elution volumes. This peak corresponds to free FGF ligand polypeptides that dissociates from the FGF:FGFR complex due to protein dilution during the chromatography process. As suramin is added to the mixture (FIGS. 13B-13C) a third peak corresponding to dimers of the FGF:FGFR complex is observed (identified by the letter D) while the intensity of the monomer peak (M) decreases. The intensities of the dimer and monomer peaks increase and decrease, respectively, as suramin is added in higher amounts (compare, e.g., FIG. 13B to FIG. 13C). Finally, when suramin is added at a 1:1:1 molar ratio to FGF and FGFR (FIG. 13D) only a peak corresponding to the FGF:FGFR dimers is observed. Thus, these experiments yield the surprising result that suramin can bind to and promote dimerization of

preformed FGF-FGFR complexes.

Paradoxically, however, FGFR dimers promoted by suramin are signaling incompetent. That is to say, the FGF receptor is not activated in these dimers. To demonstrate this property, experiments that are essentially identical to those described, *supra*, in Example 2 were performed to investigate suramin's ability to modulate FGF ligand-dependent activation of the FGF receptor *in vivo*. However, in these experiments, BaF3 cells were grown in the presence of suramin, rather than heparin of SOS, and contacted with FGF ligand. However, no heparin-like or SOS-like activity was observed when these cells were cultured with suramin.

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EXAMPLE 7: SULFONATED CYCLODEXTRIN PROMOTES ACTIVATION OF THE FGF RECEPTOR BY FGF IN CELLS

This examples describes experiments that investigate the ability of sulfonated β -cyclodextrin to function as an effective heparin agonists. In particular, the cell-based assay described in Example 2, supra, is used here to investigate the ability of sulfonated β -cyclodextrin to modulate FGF ligand-dependent activation of the FGF receptor in vivo.

The assay uses a BaF3 cell line which overexpresses FGFR1. This cell line has been previously described and is known in the art (see, e.g., Huang et al., J. Biol. Chem. 1995, 270:5065-5072). BaF3 cells are a lymphoid cell line, which are dependent on interleukin-3 (IL-3) for growth. Ordinarily these cells do not exhibit any response to FGF. However, when stably transfected to express an FGF receptor, the cells exhibit a dose-dependent mitogenic response to FGF ligand in the absence of IL-3. Accordingly, the growth rate of such transfected cells is useful as a measurement of FGF receptor activity in vivo. Ordinarily, because BaF3 cells express only low amounts of HSPG, soluble heparin must also be present to elicit the FGF-dependent mitogenic response observed in the transfected cells.

For the experiments described here, BaF3 cells that stably express wild-type FGFR1 (SEQ ID NO:3) were cultured according to standard methods that have been previously described (see, Huang et al., supra). 1 x 10⁴ cells were seeded in triplicate wells and grown in the presence of FGF1 ligand (50 ng/ml) and heparin (10 μg/ml) or,

30 alternatively, in the presence of various concentrations of sulfonated β-cyclodextrin (1 μΜ., 5 μΜ, 10 μΜ and 25 μΜ, respectively). The numbers of viable cells in each well were counted daily in duplicate. Control experiments were also performed in which cells were

incubated with either FGF1 ligand alone (i.e. no heparin or sulfonated β -cyclodextrin) or in factor-free medium with neither FGF ligand, heparin or cyclodextrin derivatives.

Data from these experiments are graphically presented in FIG. 15A as mean and standard deviation values. As can be seen from inspecting that figure, sulfonated β-cyclodextrin supports the FGF ligand in inducing proliferation of the BaF3 cells over expressing FGFR1 in a dose-dependent manner. As expected, the BaF3 cells grow minimally without FGF ligand or when grown in the presence of FGF ligand alone (i.e., without heparin or sulfonated β-cyclodextrin).

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To verify that the effect of sulfonated β -cyclodextrin observed in FIG. 15A is actually due to activation of the FGF receptor, experiments were conducted that examined the capacity of heparin and β -cyclodextrin to stimulate kinase activity of FGF receptor in living cells. See, Mohammadi *et al.*, Science 1997, 276:955-960 for a detailed description of such experiments.

Briefly, BaF3 cells over-expressing FGFR were stimulated for five minutes with FGF1 ligand (50 ng/ml), heparin (10 μ g/ml) and/or sulfonated β -cyclodextrin 5 or 25 μ M). The cells were then lysed. Their proteins were immunoprecipitated with antibodies to FGFR1, separated by SDS-polyacrylamide gel electrophoresis (PAGE), immunoblotted with antibodies to phosphotyrosine, and detected by autoradiography. As expected, the FGF ligand stimulated autophosphorylation of the FGF receptor when incubated with cells in the presence of heparin, whereas no autophosphorylation of the receptor is observed when the cells are incubated in the presence of FGF1 ligand alone (i.e., with no co-factors). See, the left-hand and right-hand lanes, respectively, in FIG. 15B. Incubation of cells with FGF1 ligand and sulfonated β -cyclodextrin also results in autophosphorylation of the FGF receptor, as illustrated in the middle lane of FIG. 15B.

Co-incubation of the cells with either heparin or sulfonated β-cyclodextrin also induces autophosphorylation of ERK-1 and ERK-2, two intracellular events that are dependent on the kinase activity of FGFR1 (FIG. 15C). By contrast, incubation of the cells with FGF1 alone (i.e., no co-factor) resulted in no autophosphorylation of either ERK-1 or ERK-2.

Thus, the data from these experiments demonstrate that sulfonated cyclodextrin derivatives are effective heparin agonists and increase FGF receptor activity in

cells, thereby enhancing signaling by an FGF ligand.

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REFERENCES CITED

Numerous references, including patents, patent applications and various

publications, are cited and discussed in the description of this invention. The citation and/or discussion of such references is provided merely to clarify the description of the present invention and is not an admission that any such reference is "prior art" to the invention described herein. All references cited and discussed in this specification are incorporated herein by reference in their entirety and to the same extent as if each reference was individually incorporated by reference.

APPENDIX: CRYSTAL STRUCTURE COORDINATES FOR AN FGF-FGFR-SOS TERNARY COMPLEX

```
REMARK coordinates from restrained individual B-factor refinement
     REMARK refinement resolution: 25 - 2.6 A
15
     REMARK starting r= 0.2409 free_r= 0.2774
                        r= 0.2408 free_r= 0:2778
     REMARK final
                                                       0.809
                                                                target= 1.5 %
     REMARK B rmsd for bonded mainchain atoms=
                                                               targer= 2.0
     REMARK B rmsd for bonded sidechain atoms= 1.077
                                                               target= 2.0
     REMARK B rmsd for angle mainchain atoms=
                                                      1.458
20
     REMARK B rmsd for angle sidechain atoms=
                                                      1.726
                                                              target= 2.5 .
     REMARK wa= 2.05842
      REMARK rweight=0.148674
     REMARK target= mlf steps= 30
      REMARK sg= P2(1)2(1)2(1) a= 64.193 b= 122.374 c= 219.490
25
     REMARK alpha= 90.000 beta= 90.000 gamma= 90.000
     REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param REMARK parameter file 2 : CNS_TOPPAR:dna-rna.param
      REMARK parameter file 3
                                  : CNS TOPPAR:water_rep.param
      REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : SCR_par.txt
      REMARK parameter file 4
30
      REMARK molecular structure file: 353sos.mtf
      REMARK input coordinates: sos_19X.pdb
      REMARK anomalous f' f' library: anom_se.lib
      REMARK reflection file= 353sos.hklt
35
      REMARK ncs= restrain ncs file= ncs.def
      REMARK B-correction resolution: 6.0 - 2.6
      REMARK initial B-factor correction applied to fobs :
                        0.444 B22= -18.604 B33= 18.161
      REMARK
                B11=
                                       0.000 B23=
                                                      0.000
40
                B12=
                        0.000 B13=
      REMARK
      REMARK B-factor correction applied to coordinate array B:
                                                                            -0.119
      REMARK bulk solvent: density level= 0.355606 e/A^3
      REMARK B-factor= 25.0325 A^2
      REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 54084(100.0%)
45
      REMARK number of unobserved reflections (no entry or |F|=0): 2070(3.8%) REMARK number of reflections rejected: 0(0.0%)
      REMARK total number of reflections used: 52014 (96.2%)
      REMARK number of reflections in working set: 49400 (91.3%)
50
```

2614 (4.8%)

REMARK number of reflections in test set: 64.193 122.374 219.490 90.00 90.00 90.00 P 21 21 21 REMARK FILENAME="sos_19XB.pdb" REMARK DATE:02-Jan-01 22:56:51 created by user: mohammad REMARK VERSION: 0.5 MOTA C GLY 15 27.348 22.092 34.405 1.00 44.79 26.719 ATOM 2 0 GLY 21.151 34.910 15 1.00 44.68 15 1.00 45.47 MOTA 3 N GLY 28.399 20.552 32.735 10 MOTA 4 CA GLY 15 27.996 27.508 21.955 33.041 1.00 45.26 23.265 MOTA 5 N HIS 16 35.008 1.00 44.16 MOTA CA HIS 16 26.922 23.521 36.309 1.00 44.70 24.898 CB HIS 16 MOTA 7 27.347 36.823 1.00 46.71 CG HIS MOTA 8 16 27.132 25.085 38.293 1.00 48.88 15 9 CD2 HIS 16 27.845 25.774 39.217 1.00 50.20 MOTA 24.528 10 MOTA ND1 HIS 16 26.066 38.967 1.00 49.77 MOTA 11 CE1 HIS 16 26.134 24.862 40.244 1..00 51.31 27.204 25.618 MOTA 12 NE2 HIS 16 40.423 1.00 51.37 MOTA 13 С HIS 16 25.390 23.465 36.197 1.00 43.88 20 14 24.774 MOTA 0 HIS 16 24.238 35.460 1.00 42.88 MOTA 15 N PHE CA PHE N PHE 17 24.782 22.546 36.933 1.00 43.17 MOTA 17 23.337 22.411 1.00 42.70 16 36.902 MOTA 17 CB PHE 17 22.890 21.409 37.974 1.00 41..54 MOTA 18 CG PHE 17 23.093 21.892 39.387 1.00 40.76 . 17 25 CD1 PHE MOTA 19 22.077 22.568 40.060 1.00 40.09 MOTA 20 CD2 PHE 17 24.310 21.702 40.033 1.00 39.89 22.268 MOTA 21 CE1 PHE 17. 23.047 41.350 1.00 38.94 MOTA 22 CE2 PHE 17 24.509 22.179 41.323 1.00 39.80 23 22.855 1.00 39.26 MOTA CZ PHE 17 23.483 41.982 .30 24 22.638 23.763 MOTA С PHE 17 37.103 1.00 42.76 36.554 MOTA 25 0 PHE 17 21.564 23.987 1.00 42.49 18 ATOM 26 N LYS 23.255 24.653 37.885 1.00 43.04 MOTA 27 CA LYS 18 22.723 25.999 38.164 1.00 43.34 LYS LYS 26.796 26.664 28 23.691 MOTA CB 18 39.045 1.00 44.23 35 . ATOM 29 CG 23.573 18 40.536 1.00 46.77 MOTA 30 CD LYS 18 24.665 27.522 1.00 48.25 41.186 CE LYS **ATOM** 31 18 24.722 27.347 42.705 1.00 49.83 27.997 MOTA 32 18 25.938 43.302 1.00 50.55 33 . C MOTA LYS 18 22.561 26.849 36.904 1.00 42.94 40 . ATOM 34. 0 LYS 18 21.584 27.583 36.749 1.00 42.85 26.782 27.557 1.00 42.59 1.00 41.91 **ATOM** 35 N ASP 19 23.573 36.043 CA ASP MOTA 36 19 23.620 34.802 MOTA 37 CB. ASP 19 24.889 27.254 33.989 1.00 43.71 26.166 27.577 ATOM 38 CG ASP 19 1.00 45.39 34.719 45 39 28.472 MOTA OD1 ASP 19 26.166 35.595 1.00 47.08 26.933 MOTA 40 OD2 ASP 19 27.183 34.385 1.00 46.25 · 19 27.287 MOTA 41 С ASP 22.470 33.855 1.00 40.44 1.00 40.25 1.00 39.00 ATOM 42 0 ASP 19 21.809 26.248 33.933 22.248 32.907 ATOM 43 N PRO 20 28.213 50 CD ATOM 44 PRO 20 23.072 29.397 32.620 1.00 38.79 31.914 MOTA 45 CA PRO 20 21.182 28.083 1.00 37.50 MOTA 46 CB PRO 20 21.096 29.475 31.274 1.00 37.48 20 . MOTA 47 CG PRO 22.058 30.337 32.054 .1.00 38.29 . 20 ATOM . 48 С PRO 21.679 27.078 30.897 1.00 36.29 55 26.862 26.480 1.00 35.46 1.00 35.82 ATOM 49 PRO 20 22.880 30.768 50 ATOM N LYS 21 20.760 30.160 MOTA 51 CA LYS 21 21.140 25.515 29.155 1.00 35.99 MOTA 52 CB LYS 21 20.914 24.078 29.674 1.00 36.49 MOTA 53 CG LYS 21 21.838 23.662 30.818 1.00 37.97 60 MOTA 54 CD LYS 21 21.583 22.233 31.306 1.00 39.15 55 MOTA CE LYS 21 22.452 21.932 32.533 1.00 40.16 56 20.529 33.055 ATOM NZ LYS 21 22.361 1.00 41.59

	ATOM	57	С	LYS	.21	20.340	25.727	27.884	1.00 35.42
•	MOTA	58	0	LYS	21	19.281	26.346	27.904	1.00 35.74
	ATOM	59	N	ARG	22	20.872	25.229	26.774	1.00 34.75
	ATOM	60	CA	ARG	22	20.176	25.294	25.501	1.00 34.07
5	ATOM	61	СВ	ARG	. 22	21.101	25.797	24.396	1.00 35.29
•	ATOM	62	CG	ARG	22	21.343	27.292	24.405	1.00 37.78
	ATOM	63	CD	ARG	22	22.090	27.710	23.148	1.00 40.24
		64	NE	ARG	22	23.513	27.924	23.380	1.00 43.27
	MOTA				22	24.029	29.059	23.845	1.00 45.68
10	ATOM	65	CZ	ARG		23.229	30.087	24.127	1.00 45.61
10	ATOM	66		ARG	22				1.00 46.18
	ATOM	67		ARG	22	25.345	29.171	24.028	
	MOTA	68	С	ARG	22	19.753	23.853	25.216	1.00 32.72
	ATOM	69	0	ARG	22	20.498	22.913	25.495	1.00 32.82
	ATOM	70	N	LEU	23	18.549	23.669	24.695	1.00 30.88
15	ATOM	71	ÇA	LEU	23	18.091	22.332	24.380	1.00 29.33
	ATOM	72	CB	LEU	23	16.691	22.110	24.936	1.00 27.76
	ATOM	.73	CG	LEU	23	16.710	21.842	26.438	1.00 27.28
	ATOM	74	CD1	LEU	23	15.317	21.643	26.964	1.00 27.57
	ATOM	75		LEU	23	17.536	20.585	26.696	1.00 28.42
20	ATOM	76	c	LEU	23	18.112	22.126	22.878	1.00 28.98
20	ATOM	77	õ	LEU	23	17.254	22.627	22.159	1.00 29.13
	ATOM	78	И	TYR	24	19.124	21.396	22.419	.1.00 28.51
		79	CA	TYR	24	19.314	21.083	21.010	1.00 28.12
	MOTA					20.804	20.847	20.769	1.00 26.44
25	ATOM	80	CB	TYR	24	21.197	20.462	19.366	1.00 25.39
25	ATOM	81	CG	TYR	24		19.146	18.916	1.00 25.38
•	MOTA	82		TYR	24	21.080			1.00 23.38
	MOTA	83	CE1		24	21.504	18.782	17.640	
	ATOM	84		TYR	24	21.739	21.405	18.499	1.00, 25.53
	ATOM	85	CE2		24	22.161	21.055	17.228	1.00 25.30
30	MOTA	86	CZ	TYR	24	22.045	19.746	16.806	1.00 25.20
	MOTA	87	ОН	TYR	24	22.491	19.421	15.553	1.00 24.70
	ATOM	88	С	TYR	24	18.495	19.841	20,651	1.00 28.56
	ATOM	89	0	TYR	24	18.726	18.758	21.188	1.00 28.69
	ATOM .	90	N	CYS	25	17.531	20.003	19.752	1.00 28.93
35	ATOM	91	CA	CYS	25	16.691	18.885	19.338	1.00 29.34
	ATOM	92	CB	CYS	25	15.371	19.407	18.786	1.00 28.57
	ATOM	93	SG	CYS	25	14.151	18.130	18.521	1.00 27.13
	ATOM	94	c	CYS	25	17.377	18.019	18.290	1.00 29.52
	ATOM	95	ō	CYS	25	17.904	18.527	17.311	1.00 29.96
40	ATOM	96	N	LYS	. 26	17.363	16.711	18.499	1.00 30.38
40	ATOM	97	CA	LYS	26	17.999	15.775	17.582	1.00 31.27
		98	CB	LYS	26	17.907	14.363	18.157	1.00 29.40
	ATOM	99	CG	LYS	26	18.580	13.292		1.00 27.53
	ATOM			LYS	26	18.601	11.990	18.104	1.00 25.63
45	ATOM	100	CD		26	19.451	10.965	17.421	1.00 24.68
45	ATOM	101	CE	LYS		18.924	10.707	16.055	1.00 25.40
	MOTA	102	ΝZ	LYS	·26				
	ATOM	103	С	LYS	26	17.341	15.816	16.213	
	MOTA	104	0	LYS	26	17.962	15.515	15.192	1.00 34.06
	ATOM	105	N	. ASN	27	16.080	16,212	16.198	1.00 34.37
50	MOTA	106	CA	ASN	27 ·	15.319	16.276	14.964	1.00 35.49
	MOTA	107	CB	ASN	27.	13.840	16.054	15.283	1.00 36.29
	ATOM	108	CG	ASN	27	13.020	. 15.786	14.051	1.00 37.55
	ATOM	109		ASN	27	13.468	15.086	13.141	1.00 37.50
	ATOM	110		ASN	27	11.799	16.320	14.019	1.00 37.52
55	MOTA	111	C	ASN	27	15.511	17.586	14.191	1.00 35.42
55	ATOM	112	ŏ	ASN	27	14.691	18.494	14.273	1.00 35.77
	ATOM	113	N	GLY	28	16.605	17.676	13.442	1.00 35.14
	ATOM	114	CA	GLY	28	16.860	18.865	12.657	1.00 34.17
						17.881	19.807	13.257	1.00 34.17
60	MOTA	115	C	GLY	28 ·		20.707	12.581	1.00 34.08
60	ATOM	116	0	GLY	28	18.360			1.00 34.14
	ATOM	117	N	GLY	29	18.211	19.612	14.526	
	ATOM	118	CA	GLY	29	19.182	20.477	15.170	1.00 33.68

ATOM 121 N PHE 30 16.755 23.175 16.307 1.00 32.91 ATOM 122 CA PHE 30 16.755 23.175 16.307 1.00 32.91 ATOM 123 CB PHE 30 16.755 23.175 16.307 1.00 32.91 ATOM 123 CG PHE 30 15.081 23.233 15.879 1.00 31.65 ATOM 125 CD1 PHE 30 15.081 23.415 14.413 1.00 30.62 ATOM 125 CD1 PHE 30 15.081 23.415 14.413 1.00 30.62 ATOM 125 CD1 PHE 30 15.081 23.415 14.413 1.00 30.62 ATOM 125 CD1 PHE 30 15.081 23.415 14.413 1.00 30.62 ATOM 127 CE1 PHE 30 14.552 22.503 12.251 1.00 30.75 ATOM 127 CE1 PHE 30 14.552 22.503 12.251 1.00 30.75 ATOM 128 CE2 PHE 30 14.974 24.866 12.471 1.00 30.76 ATOM 129 CZ PHE 30 16.791 23.313 17.817 1.00 30.76 ATOM 130 C PHE 30 16.791 23.313 17.817 1.00 32.25 ATOM 130 CP PHE 30 16.791 23.313 17.817 1.00 32.25 ATOM 131 CP PHE 30 16.791 23.313 17.817 1.00 32.25 ATOM 133 CP PHE 30 16.791 23.313 17.817 1.00 32.25 ATOM 133 CP PHE 31 17.144 24.500 18.290 1.00 32.25 ATOM 133 CP PHE 31 17.144 24.500 18.290 1.00 32.25 ATOM 134 CB PHE 31 17.146 24.772 19.722 1.00 32.25 ATOM 135 CP PHE 31 19.591 25.580 19.855 1.00 31.32 ATOM 136 CP PHE 31 20.230 24.772 20.796 1.00 31.32 ATOM 136 CP PHE 31 20.230 24.772 20.796 1.00 30.62 ATOM 137 CP PHE 31 20.230 24.772 20.796 1.00 30.62 ATOM 137 CP PHE 31 20.342 26.095 18.795 1.00 30.62 ATOM 137 CP PHE 31 20.342 26.095 18.795 1.00 30.62 ATOM 137 CP PHE 31 20.342 26.095 18.795 1.00 30.62 ATOM 134 CP PHE 31 22.332 25.006 19.629 1.00 29.43 ATOM 140 CP PHE 31 22.332 25.006 19.629 1.00 39.89 ATOM 141 CP PHE 31 22.332 25.006 19.629 1.00 39.89 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 34.48 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 34.08 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.479 1.00 33.09 ATOM 140 CP PHE 31 15.086 25.897 19.00 30.00 25.40 ATOM 140 CP PHE 31 15.086 25.897 19.00 30.00 25.40 A		ATOM	119	С	GLY	29	18.650	21.850	15.550	1.00 33.77
ATOM 123 CB PHE 30 16.755 23.175 16.307 1.00 32.13 ATOM 124 CG PHE 30 15.28B 23.233 15.879 1.00 31.86 ATOM 125 CD1 PHE 30 15.28B 23.233 15.879 1.00 30.62 ATOM 126 CD2 PHE 30 15.081 23.415 14.413 1.00 30.62 ATOM 127 CE1 PHE 30 14.764 22.332 13.666 1.00 30.76 ATOM 127 CE1 PHE 30 14.764 22.332 13.666 1.00 30.76 ATOM 128 CE2 PHE 30 14.552 22.503 12.251 1.00 30.72 ATOM 129 CZ PHE 30 14.974 24.866 12.471 1.00 30.76 ATOM 130 C PHE 30 14.656 23.777 11.676 1.00 30.72 ATOM 131 O PHE 30 16.502 22.361 18.540 1.00 32.25 ATOM 131 O PHE 31 17.144 24.500 18.290 1.00 32.25 ATOM 132 N PHE 31 17.148 24.772 19.722 1.00 32.26 ATOM 134 CB PHE 31 17.18B 24.772 19.722 1.00 32.26 ATOM 135 CG PHE 31 19.591 25.580 19.855 1.00 31.32 ATOM 136 CD1 PHE 31 20.342 26.095 18.795 1.00 30.64 ATOM 136 CD1 PHE 31 20.342 26.095 18.795 1.00 30.64 ATOM 137 CD2 PHE 31 20.342 26.095 18.795 1.00 30.62 ATOM 138 CE2 PHE 31 21.596 24.484 20.687 1.00 29.43 ATOM 140 CZ PHE 31 21.596 24.484 20.687 1.00 29.43 ATOM 140 CZ PHE 31 21.596 24.484 20.687 1.00 29.43 ATOM 140 CZ PHE 31 21.596 24.484 20.687 1.00 29.43 ATOM 140 CZ PHE 31 21.596 24.484 20.687 1.00 30.64 ATOM 140 CZ PHE 31 21.596 24.4896 21.895 1.00 30.62 ATOM 144 C PHE 31 15.782 25.157 20.177 1.00 33.39 ATOM 146 CG PHE 31 15.862 58.87 19.479 1.00 33.38 ATOM 146 CG PHE 31 21.206 24.649 21.325 1.00 33.48 ATOM 146 CG PHE 31 15.862 58.87 19.479 1.00 33.38 ATOM 148 CD2 1888 31 15.862 58.87 19.479 1.00 33.39 ATOM 148 CD2 1888 31 15.862 58.87 19.479 1.00 33.39 ATOM 148 CD2 1888 31 15.862 58.87 19.479 1.00 33.328 ATOM 148 CD2 1888 31 15.862 58.87 19.479 1.00 33.38 ATOM 148 CD2 1888 31 15.862 58.87 19.479 1.00 33.39 ATOM 148 CD2 1888 31 18.586 62.3790 25.689 1.00 33.344 ATOM 155 CB ARG 33 13.045 27.294 21.395 1.00 33.448 ATOM 156 CB LEU 32 12.331 24.996 23.104 1.00 33.25 ATOM 157 C ARG 33 13.662 31.570 19.369 1.00 33.374 ATOM 156 CB ARG 33 13.065 27.294 25.399 1.00 33.393 ATOM 157 C ARG 33 13.662 31.577 19.369 1.00 33.373 ATOM 156 CB ARG 33 13.662 31.577 19.369 1.00 33.393 ATOM 157 C ARG 33 11.677 19.389 20.513 1.		ATOM	120		GLY ·	29	19.382		15.513	1.00 34.35
5 ATOM 123 CB PHE 30 15.288 23.233 15.879 1.00 31.62 ATOM 124 CG PHE 30 15.081 23.415 14.413 1.00 30.62 ATOM 125 CD1 PHE 30 14.764 22.332 13.606 1.00 30.76 ATOM 126 CD2 PHE 30 14.764 22.332 13.606 1.00 30.76 ATOM 127 CE1 PHE 30 14.974 22.332 13.606 1.00 30.76 ATOM 128 CE2 PHE 30 14.974 24.866 12.471 1.00 30.76 ATOM 129 CZ PHE 30 14.974 24.866 12.471 1.00 30.76 ATOM 130 C PHE 30 16.791 23.313 17.817 1.00 30.22 ATOM 131 O PHE 30 16.791 23.313 17.817 1.00 32.26 ATOM 131 O PHE 30 16.791 23.313 17.817 1.00 32.26 ATOM 133 CA PHE 31 17.144 24.500 18.590 1.00 32.25 15 ATOM 133 CA PHE 31 17.144 24.500 18.290 1.00 32.25 ATOM 135 CG PHE 31 19.332 25.927 20.004 1.00 32.35 ATOM 136 CD1 PHE 31 17.149 24.500 18.290 1.00 32.25 ATOM 137 CD2 PHE 31 19.591 25.580 19.855 10.00 30.62 ATOM 138 CE1 PHE 31 19.591 25.580 19.855 10.00 31.32 ATOM 138 CE1 PHE 31 20.230 24.772 20.796 1.00 30.62 ATOM 138 CE2 PHE 31 20.530 24.772 20.796 1.00 30.62 ATOM 139 CE2 PHE 31 21.596 24.844 20.667 1.00 29.89 ATOM 140 CZ PHE 31 22.332 25.006 19.625 10.00 29.89 ATOM 141 C PHE 31 15.782 25.812 18.679 1.00 29.89 ATOM 141 C PHE 31 15.782 25.812 18.679 1.00 33.39 ATOM 144 CA LEU 32 11.576 23.812 18.679 1.00 33.39 ATOM 144 CA LEU 32 11.270 23.743 22.1071 1.00 33.00 ATOM 147 CD LEU 32 11.270 23.743 22.2844 1.00 33.04 ATOM 148 CD2 LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 146 CG LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 147 CD LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 148 CD2 LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 149 CD LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 150 O LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 150 O LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 150 O LEU 32 11.270 23.743 22.844 1.00 33.04 ATOM 150 O LEU 32 11.270 23.743 23.790 25.099 1.00 33.74 ATOM 150 O LEU 32 11.270 23.743 23.790 25.099 1.00 33.74 ATOM 160 C ARG 33 13.866 32.004 23.991 1.00 33.64 ATOM 150 O LEU 32 14.288 26.481 22.315 1.00 33.64 ATOM 150 O LEU 32 14.288 26.481 22.315 1.00 33.64 ATOM 150 O LEU 32 12.284 1.00 33.55 1.00 33.991 ATOM 160 C ARG 33 10.574 28.89 23.90		ATOM								
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ATOM 159 NH2 ARG 33 11.938 31.581 16.135 1.00 32.74 ATOM 160 C ARG 33 11.672 29.128 22.460 1.00 35.77 ATOM 161 O ARG 33 10.574 28.771 22.031 1.00 35.95 ATOM 162 N ILE 34 11.817 29.948 23.490 1.00 36.85 ATOM 163 CA ILE 34 10.678 30.507 24.195 1.00 38.11 ATOM 164 CB ILE 34 10.791 30.237 25.715 1.00 37.62 ATOM 165 CG2 ILE 34 9.704 30.988 26.461 1.00 36.83 ATOM 166 CG1 ILE 34 10.698 28.730 25.979 1.00 36.70 ATOM 167 CD1 ILE 34 10.698 28.730 25.979 1.00 36.70 ATOM 168 C ILE 34 10.698 28.730 25.979 1.00 36.70 ATOM 169 O ILE 34 10.656 32.004 23.921 1.00 38.77 ATOM 169 O ILE 34 11.515 32.738 24.397 1.00 38.44 ATOM 170 N HIS 35 9.678 32.444 23.137 1.00 40.65 ATOM 171 CA HIS 35 9.538 33.853 22.774 1.00 42.57 ATOM 172 CB HIS 35 8.638 33.994 21.543 1.00 42.64 55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.70 ATOM 175 ND1 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.66 ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 9.819 32.220 18.551 1.00 44.53	40									
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ATOM 162 N ILE 34 11.817 29.948 23.490 1.00 36.85 ATOM 163 CA ILE 34 10.678 30.507 24.195 1.00 38.11 ATOM 164 CB ILE 34 10.791 30.237 25.715 1.00 37.62 ATOM 165 CG2 ILE 34 9.704 30.988 26.461 1.00 36.83 ATOM 166 CG1 ILE 34 10.698 28.730 25.979 1.00 36.70 ATOM 167 CD1 ILE 34 10.892 28.345 27.430 1.00 37.36 ATOM 168 C ILE 34 10.656 32.004 23.921 1.00 38.77 ATOM 169 O ILE 34 11.515 32.738 24.397 1.00 38.77 ATOM 170 N HIS 35 9.678 32.444 23.137 1.00 40.65 ATOM 171 CA HIS 35 9.538 33.853 22.774 1.00 42.57 ATOM 172 CB HIS 35 9.538 33.853 22.774 1.00 42.64 55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 176 CE1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65			160	C	ARG	33				
45 ATOM 163 CA ILE 34 10.678 30.507 24.195 1.00 38.11 ATOM 164 CB ILE 34 10.791 30.237 25.715 1.00 37.62 ATOM 165 CG2 ILE 34 9.704 30.988 26.461 1.00 36.83 ATOM 166 CG1 ILE 34 10.698 28.730 25.979 1.00 36.70 ATOM 167 CD1 ILE 34 10.892 28.345 27.430 1.00 37.36 37.36 ATOM 168 C ILE 34 10.656 32.004 23.921 1.00 38.77 ATOM 169 O ILE 34 11.515 32.738 24.397 1.00 38.44 ATOM 170 N HIS 35 9.678 32.444 23.137 1.00 40.65 ATOM 171 CA HIS 35 9.538 33.853 22.774 1.00 42.67 ATOM 173 CG HIS 35 8.638 33.994 21.543 1.00 42.64 55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 9.819 32.220 18.551 1.00 44.66 ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65					•					
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ATOM 165 CG2 ILE 34 9.704 30.988 26.461 1.00 36.83 ATOM 166 CG1 ILE 34 10.698 28.730 25.979 1.00 36.70 ATOM 167 CD1 ILE 34 10.892 28.345 27.430 1.00 37.36 50 ATOM 168 C ILE 34 10.656 32.004 23.921 1.00 38.77 ATOM 169 O ILE 34 11.515 32.738 24.397 1.00 38.44 ATOM 170 N HIS 35 9.678 32.444 23.137 1.00 40.65 ATOM 171 CA HIS 35 9.538 33.853 22.774 1.00 42.57 ATOM 172 CB HIS 35 8.638 33.994 21.543 1.00 42.57 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65	45									
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50 ATOM 168 C ILE 34 10.656 32.004 23.921 1.00 38.77 ATOM 169 O ILE 34 11.515 32.738 24.397 1.00 38.44 ATOM 170 N HIS 35 9.678 32.444 23.137 1.00 40.65 ATOM 171 CA HIS 35 9.538 33.853 22.774 1.00 42.57 ATOM 172 CB HIS 35 8.638 33.994 21.543 1.00 42.64 55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.66 ATOM 176 CE1 HIS </td <td></td>										
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ATOM 171 CA HIS 35 9.538 33.853 22.774 1.00 42.57 ATOM 172 CB HIS 35 8.638 33.994 21.543 1.00 42.64 55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 10.524 33.338 18.512 1.00 44.66 ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65						34	11.515	32.738		1.00 38.44
ATOM 172 CB HIS 35 8.638 33.994 21.543 1.00 42.64 55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 10.524 33.338 18.512 1.00 44.66 ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65		ATOM								
55 ATOM 173 CG HIS 35 9.225 33.423 20.290 1.00 43.75 ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 10.524 33.338 18.512 1.00 44.66 ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65										
ATOM 174 CD2 HIS 35 9.000 32.248 19.653 1.00 43.70 ATOM 175 ND1 HIS 35 10.185 34.082 19.551 1.00 44.37 ATOM 176 CE1 HIS 35 10.524 33.338 18.512 1.00 44.66 ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65		-								
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ATOM 177 NE2 HIS 35 9.819 32.220 18.551 1.00 44.53 60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65										
60 ATOM 178 C HIS 35 8.939 34.681 23.902 1.00 43.65										
	60									
		ATOM	179		HIS					1.00 43.83
ATOM 180 N PRO 36 9.347 35.952 24.009 1.00 45.01				N		36	9.347	35.952	24.009	1.00 45.01

	ATOM	181	CD	PRO	36	10.350	36.645	23.180	1.00 45.93
	ATOM	182	CA	PRO	36	8.832	36.842	25.052	1.00 45.83
	MOTA	183	CB	PRO	36	9.462	38.184	24.700	1.00 45.55
_	MOTA	184	CG	PRO	36	10.755	37.792	24.073	1.00 46.12
5	MOTA	185	С.	PRO	36	7.305	36.916	25.046	1.00 46.80
	MOTA	186	Ο.		36	6.689	37.107	26.091	1.00 47.50
	ATOM	187	N	ASP	37	6.700	36,752	23.873	1.00 47.49
	ATOM	188	CA	ASP	37	5.250	36.824	23.745	1.00 48.34
	MOTA	189	СВ	ASP	37	4.866	37.314	22.339	1.00 49.10
10	MOTA	190	CG	ASP	37	5.081	36,254	21.252	1.00 50.21
	ATOM	191		ASP	37	4.340	35.247	21.242	1.00 50.76
	ATOM	192		ASP	37	5.983	36.429	20.401	1.00 49.91
	ATOM	193	C	ASP	3. 37	4.524	35.515	24.044	1.00 48.65
	· ATOM	194	ŏ	ASP	3 <i>7</i>	3.301	35.438	23.913	1.00 48.42
15	ATOM	195	Й	GLY	38	5.266	34.485	24.438	1.00 48.59
13							33.213	24.744	1.00 48.28
	MOTA	196	CA	GLY	38	4.631			
	ATOM	197	C	GLY	38 .	4.685	32.156	23.653	1.00 47.65
	MOTA	198	0	GLY	38	4.202	31.043	23.842	1.00 47.29
~~	MOTA	199	N	ARG	39	5.268	32.496	22.508	1.00 47.21
20	MOTA	200	CA	ARG	39	5.381	31.545	21.408	1.00 46.53
	ATOM	201	CB	ARG	39	5.535	32.269	20.070	1.00 46.19
	MOTA	202	CG	ARG	39	4.259	32.830	19.488	1.00 45.95
	MOTA	203	CD	ARG	39	4.559	33.524	18.175	1.00 46.28
	ATOM	204	NE	ARG	39	5.588	34.547	18:340	1.00 45.77
25	ATOM	205	CZ	ARG	39	6.647	34.674	17.547	1.00 46.38
	ATOM	206	NH1	ARG	39	7.533	35.636	17.780	1.00 46.10
	MOTA	207	NH2	ARG	39	6.822	33.836	16.524	1.00 46.14
	ATOM	. 208	C	ARG	39 ·	6.575	30.619	21.596	1.00 45.86
	ATOM	209	ŏ	ARG	39	7.654	31.060	21.991	1.00 46.25
30	. ATOM	210	N	VAL	40	6.377	29.338	21.308	1.00 44.53
-	ATOM	211	CA	VAL	4.0	7.446	28.354	21.431	1.00 43.43
	. ATOM	212	CB	VAL	40	7.111	27.264	22.470	1.00 42.18
•	ATOM	2.13	CG1		40	8.268	26.287	22.582	1.00 41.55
	· ATOM	214	CG2		40	6.835	27.891	23.808	1.00 41.76
35				VAL	40	7.713	27.660	20.100	1.00 43.16
20	MOTA	215	С						
	ATOM	216	0	VAL	40	6. . 793	27.152	19.458	1.00 43.30
	ATOM	217	N	ASP	41	8.973	27.644	19.687	1.00 42.42
	ATOM	218	CA	ASP	41.	9.364	26.986	18.446	1.00 41.97
40	ATOM	219	CB	ASP	41	9.053	27.875	17.240	1.00 40.91
40	ATOM	220	CG	ASP	41	9.874	29.148	17.219	1.00 41.31
	ATOM	221		ASP	41	9.666	29.969	16.304	1.00 41.93
	ATOM	222	OD2	ASP	41	10.732	29.336	18.108	1.00 41.72
	ATOM	223.	С	ASP	41.	10.859	26.670	18.507	1.00 41.82
	ATOM	224	0	:ASP	41	11.461	26.691	19.583	1.00 41:15
45	ATOM	225	N	GLY	42	11.454	26.376	17.358	1.00 41.58
	ATOM	226	CA	GLY	42	12.873	26.076	17.339	1.00 41.56
	ATOM	227	С	GLY	42	13.650	26.897	16.324	1.00 41.64
	ATOM	228	0	GLY	42	13.092	27.396	15.349	1.00 41.88
	ATOM	229	Ν.	VAL	43	14.943	27.059	16.574	1.00 41.45
50	ATOM	230	CA	VAL	43	15.819	27.780	15.666	1.00 41.09
	ATOM	231	CB	VAL	43	15.923	29.266	16.002	1.00 41.11
	ATOM	232		VAL	43	14.600	29.927	15.702	1.00 41.85
	ATOM	233		VAL	43	16.320	29.460	17.456	1.00 40.06
	ATOM	234		VAL	43	17.189	27.162	15.741	1.00 40.00
55			C .					16.756	1.00 41.13
JJ	MOTA	235	0	VAL	43	17.559	26.585		
	ATOM	236	N	ARG	44	17.941	27.279	14.656	1.00 41.51
	ATOM	237	CA	ARG	44	19.267	26.705	14.603	1.00 41.23
	ATOM	238	CB	ARG	44	19.535	26.193	13.201	1.00 39.47
.	ATOM	239	CG	ARG	44	18.788	24.906	12.906	1.00 38.20
60	ATOM	240	CD	ARG	44	18.874	24.564	11.455	1.00 37.03
	ATOM	241	NE	ARG	44	18.455	23.198	11.197	1.00 36.73
	ATOM	242	CZ	ARG	44	17.801	22.821	10.104	1.00 36.87

						17 400	22 716	9.174	1.00 36.61
	ATOM	243	NH1		44	17.486	23.716	9.930	1.00 35.75
	ATOM	244	NH2		44	17.477	21.549		
	ATOM .	245	С	ARG	44	20.363	27.641	15.049	1.00 42.52
	MOTA	246	0	ARG	44	21.406	27.190	15.501	1.00 43.57
5	MOTA	247	N	GLU	45	20.127	28.942	14.949	1.00 43.99
	ATOM	248	CA	GLU	45	21.130	29.921	15.356	1.00 45.63
	ATOM	249	CB	GLU	.45	20.662	31.329	14.978	1.00 46.78
	ATOM	250	CG	GLU	45	21.697	32.412	15.235	1.00 48.93
	ATOM	251	CD	GLU	45	22.977	32.197	14.438	1.00 50.48
10	ATOM	252	OE1		.45	22.904	32.181	13.184	1.00 51.97
10	ATOM	253	OE2		45	24.053	32.045	15.065	1.00 50.49
		254		GLU	45	21.421	29.856	16.856	1.00 45.57
	ATOM		C			20.590	30.238	17.673	1.00 45.09
	ATOM	255	0	GLU	45			17.201	1.00 46.06
	MOTA	256	N	LYS	46	22.614	29.379		
15	ATOM	257	CA	LYS	46	23.030	29.247	18.592	1.00 46.74
	ATOM	258	CB	LYS	46	24.396	28.553	18.660	1.00 46.79
	ATOM ·	259	CG	LYS	46	25.061	28.592	20.038	1.00 47.95
	ATOM	260	CD	LYS	46	25.708	27.261	20.403	1.00 48.10
	ATOM	261	CE	LYS	46	26.700	27.403	21.553	1.00 48.89
20	ATOM	262	NZ	LYS	46	27.971	28.065	21.117	1.00 [.] 49.06
	ATOM	263	С	LYS	46	23.077	30.565	19.367	1.00 47.09
	ATOM	264	ŏ	LYS	46	23.012	30.572	20.603	1.00 47.49
}		265	N	SER	47	23.170	31.679	18.648	1.00 46.92
	MOTA			SER	47	23.242	32.990	19.285	1.00 46.51
25	ATOM	266	CA		47	24.067	33.946	18.420	1.00 46.05
25	MOTA	267	CB.	SER			34.109	17.137	1.00 46.10
•	ATOM	268	OG	SER	47	23.487			1.00 46.68
	MOTA	269	С	SER	47	21.887	33.626	19.596	
	MOTA	270	0	SER	47	21.831	34.697	20.204	1.00 46.55
	ATOM	271	N	ASP	48	20.798	32.987	19.176	1.00 46.40
30	ATOM.	272	CA	ASP	48	19.47.7	33.537	19.455	1.00 46.21
	ATOM	273	CB	ASP	48	18.381	32.591	18.967	1.00 46.23
	ATOM	274	CG	ASP	48 '	17.003	33.219	19.042	1.00 46.68
	ATOM	275		ASP	48	16,327	33.313	17.998	1.00 47.11
•	ATOM	276		ASP	48	16.595	33.626	20.147	1.00 47.69
35	ATOM	277	c	ASP	. 48	19.374	33.736	20.968	1.00 46.01
33	ATOM	278	ŏ	ASP	48	19.760	32.866	21.750	1.00 46.53
		279		PRO	49	18.857	34.891	21.403	1.00 45.50
	ATOM		И		49	18.476	36.072	20.608	1.00 45.51
	ATOM	280	CD	PRO		18.731		22.838	1.00 45.10
40	ATOM	281	CA	PRO	49			22.879	1.00 45.08
40	ATOM	282	CB	PRO	49	18.564	36.682		1.00 45.21
	ATOM	283	CG	PRO	49	17.772	36.942	21.629	
	ATOM	284	C	PRO	49	17.606	34.439	23.581	1.00 44.24
	MOTA	285	0	PRO	49	17.645	34.319	24.807	1.00 44.38
	MOTA	286	N	HIS	50	16.618	33.947	22.843	1.00 43.12
45	ATOM	287	CA	HIS	50	15.479	33.281	23.458	1.00 41.52
	ATOM	288	CB	HIS	50	14.210	33.653	22.704	1.00 41.66
	ATOM	289	CG	HIS	50	14.071	35.121	22.463	1.00 42.30
	ATOM	290		HIS	50	13.926	35.828	21.318	1.00 42.60
	ATOM	291		HIS	50	14.084	36.045	23.484	1.00 42.47
· 50					50	13.954	37.259	22.980	1.00 42.34
50	ATOM	292		HIS	50	13.856	37.155	21.667	1.00 42.47
	ATOM	293		HIS		15.564	31.771	23.570	1.00 40.32
	ATOM	294	C	HIS	50				1.00 40.32
	ATOM	295	0	HIS	50	14.539	31.113	23.710	
	ATOM	296	N.	ILE	51	16.769	31.215	23.505	1.00 39.52
55 .	ATOM	297	CA	ILE	51	16.923	29.766	23.630	1.00 38.51
	MOTA	298	CB	ILE	51	17.654	29.138	22.411	1.00 38.26
	ATOM	299		ILE	51	16.797	29.306	21.156	1.00 36.50
	ATOM	300		ILE	51	19.056	29.744	22.261	1.00 38.02
	ATOM	301		ILE	51	19.892	29.091	21.186	1.00 37.88
60	ATOM	302	C.	ILE	51	17.662	29.391	24.913	1.00 38.14
-	ATOM	303	o.	ILE	51	17.821	28.215	25.223	1.00 37.89
	ATOM	304	N	LYS	52	18.119	30.400	25.649	1.00 38.05
	MION	204	7.4	-10	JŁ	10.117	555		

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		ATOM	305	CA	LYS	52	18.796	30.182	26.925	1.00 38.46
		ATOM	306	CB	LYS	52	19.479	31.460	27.407	1.00 39.92
		MOTA	307	CG	LYS	52	20.464	32.041	26.428	1.00 43.21
		ATOM	308	ÇD	LYS	52	20.869	33.458	26.821	1.00 46.18
	5	ATOM	309	CE	LYS	52	21.776	34.081	25.752	1.00 47.91
		ATOM	310	NZ	LYS	52	22.998	.33.244	25.518	1.00 48.79
		ATOM	311	С	LYS	52	17.677	29.838	27.896	1.00 37.80
		ATOM	312	0	LYS	52	16.835	30.686	28.214	1.00 37.80
		ATOM	313	N	LEU	53	17.666	28.599	28.370	1.00 36.17
	10	ATOM	314	CA	LEU	53	16.620	28.150	29.266	1.00 33.73
		MOTA	315	CB	LEU	53	15.942	26.928	28.648	1.00 32.80
		MOTA	316	CG	LEU	53	15.591	27.119	27.168	1.00 31.74
		MOTA	317	CD1	LEO	53	15.106	.25.828	26.547	1.00 31.06
		ATOM	318	CD2	LEU	53	14.528	28.182	27.058	1.00 31.89
	15	MOTA	319	С	LEU	53	17.147	27.817	30.647	1.00 33.17
		MOTA	320	0	LEU	53	18.310	27.487	30.822	1.00 32.86
•		MOTA	321	N	GLN	54	16.274	27.914	31.634	1.00 32.71
		MOTA	322	CA	GLN	54	16.652	27.605	32.995	
		MOTA	323	ÇВ	GLN	54	16.363	28.802	33.896	1.00 32.34
٠ :	20	MOTA	324	CG	GLN	54	17.001	28.705	35.249	1.00 31.47
		MOTA	325	CD	GLN .	54	18.497	28.699	35.143	1.00 31.55
}		ATOM	326		GLN	54	19.068	29.545	34.465	1.00 32.74
,		ATOM	327		GLN	54	19.148	27.750	35.811	1.00 - 31.36
	~~	ATOM	328	C	GLN	54	15.827	26.400	33.432	1.00 32.20
	25	ATOM	329	0	GLN	. 54	14.624	26.511	33.648	1.00 33.12
	•	ATOM	330	И	LEU	55	16.478	25.249	33.541	1.00 31.21
	_	ATOM	331	CA	LEU	55	15.816	24.025	33.939 33.232	1.00 30.46
		ATOM	332	CB	LEU	55	16.482	22.845 23.052	31.714	1.00 29.98 1.00 29.60
		. ATOM	333	CG	LEU	55	16.557 17.358	21.971	31.048	1.00 29.73
	30	ATOM	334		LEU	55 55	15.159	23.054	31.162	1.00 29.86
		ATOM	335 336	CDZ	LEU LEU	55 55	15.933	23.034	35.450	1.00 25.00
		ATOM ATOM	337	Ö	LEU .	55 55	17.026	23.876	36.004	1.00 31.00
		ATOM	338	Ŋ	GLN .	56	14.786	23.879	36.114	1.00 31.09
	35	ATOM	339	CA	GLN	56	14.727	23.826	37.565	1.00 30.72
	<i>JJ</i>	MOTA	340	CB	GLN	56	14.075	25.125	38.060	1.00 29.53
		ATOM	341	CG	GIN	56	13.885	25.231	39.551	1.00 29.08
		ATOM	342	CD	GLN	56	15.195	25.215	40.319	1.00 29.28
		ATOM	343	OE1		56	16.022	26.117	40.180	1.00 27.65
	40	ATOM	344		GLN	56	15.383	24.185	41.147	1.00 29.56
		ATOM	345	С	GLN	56	13.938	22.610	38.049	1.00 30.75
		ATOM	346	0	GLN .	56	12.785	22.419	37.677	1.00 31.32
	;	ATOM	347	N ·	ALA	57	14.563	21.788	38.880	1.00 30.82
\		ATOM	348	CA	ALA	57	13.891	20.612	39.407	1.00 31.62
)	45	ATOM	349	CB	ALA	57	14.905	19.669	40.031	1.00 29.49
		ATOM	350	C	ALA	57	12.893	21.071	40.459	1.00 32.63
		MOTA	351	0	ALA	57	13.217	21.929	41.285	1.00 32.89
		MOTA	352	N	GLU	58	11.685	20.515	40.420	1.00 32.95
•		MOTA	353	CA	GLU	58	10.647	20.851	41.387	1.00 33.67
	50	ATOM	354	СВ	GLU	58	9.290	20.862	40.702	1.00 33.94
		ATOM	355	CG	GLU	58	8.277	21.746	41.379	1.00 34.98
		ATOM	356	CD	GLU	58	8.813	23.140	41.604	1.00 35.72
		ATOM	357	OE1		58	9.533	23.653	40.716	1.00 37.44
	<i></i>	ATOM	358	OE2		58	8.509	23.729	42.658	1.00 36.47
	55	ATOM	359	С	GLU	58	10.700	19.745	42.434	1.00 34.07
		ATOM	360	.0	GLU	58	10.379	19.938	43.605	1.00 33.94
		ATOM	361	N	GTO .	59	11.105	18.572	41.971	1.00 34.50
		ATOM	362	CA	GLU	59	11.283	17.398	42.807	1.00 34.71
	۲۵.	ATOM	363	CB	GLU	59 50	9.948	16.806	43.244	1.00 34.51
	60	ATOM	364	CG	GLU	59 50	9.123	16.202	42.170	1.00 35.87
		ATOM	365	CD	GLU	59 50	7.769 6.988	15.816 16.742	42.707	1.00 37.28
	•	ATOM	366	OFIT	GLU	59	0.300	10.742	43.031	1.00 37.78

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	ATOM	367	OE2	GLU	59	7.495	14.598	42.825	1.00 37.92
	ATOM	368	С	GLU	59	12.083	16.420	41.971	1.00 34.27
	ATOM	369	0	GLU	59	12.424	16.727	40.834	1.00 34.69
	ATOM	370	N	ARG	60	12.405	15.257	42.522	1.00 34.11
5	ATOM	371	CA	ARG	60	13.198	14.284	41.782	1.00 33.43
5					60	13.335	12.975	42.561	1.00 34.80
	MOTA	372	CB	ARG				43.384	1.00 37.91
	MOTA	373	CG	ARG	60	14.590	12.869		
	MOTA	374	CD	ARG	60	14.742	11.464	43.954	1.00 40.21
•	ATOM .	375	NE	ARG	60	14.480	10.470	42.918	1.00 44.07
10	ATOM	376	CZ	ARG	60	14.911	9.208	42.934	1.00 45.24
	MOTA	377	NH1	ARG	60	15.643	8.757	43.942	1.00 44.84
	MOTA	378	NH2	ARG	60	14.610	8.396	41.924	1.00 45.82
	ATOM ·	379	С	ARG	60	12.685	13.964	40.388	1.00 31.80
	ATOM	380	ŏ	ARG	60	11.559	13.502	40.220	1.00 31.15
15	ATOM	381	N	GLY	61	13.531	14.218	39.395	1.00. 30.60
13						13.200	13.916	38.013	1.00 29.48
	ATOM	382	ÇA	GLY	61			37.351	1.00 28.97
	MOTA	383	C	GLY	61	12.147	14.778		
	ATOM.	384	0	GLY	61	11.782	14.540	36.199	1.00 28.95
	ATOM	385	N	VAL	62	11.656	15.780	38.074	1.00 28.54
20	ATOM	386	CA	VAL	. 62	10.627	16.679	37.554	1.00 27.15
	ATOM	387	ÇВ	VAL	62 ·	9.395	16.718	38.487	1.00 25.88
}	ATOM	388	CG1	VAL	62	8.448	17.817	38.053	1.00 22.76
,	ATOM	389	·CG2		62	8.680	15.364	38.469	1.00 25.15
	ATOM	390	C	VAL	62	11.179	18.088	37.456	1.00 27.19°
25	ATOM	391	ŏ	VAL	. 62	11.647	18.636	38.448	1.00 27.64
2,5				VAL	63	11.116	18.683	36.270	1.00 26.77
	ATOM	392	N			11.619	20.040	36.095	1.00 26.70
•	ATOM	393	CA	VAL	63				1.00 26.70
•	ATOM	394	CB	LAV	63	12.911	20.057	35.236	
••	MOTA	395	CG1		63	13.946	19.123	35.822	1.00 25.10
30	ATOM	396	CG2		63	12.588	19.656	33.812	1.00 25.90
	MOTA	397	С	VAL	63	10.631	20.996	35.423	1.00 27.27
•	MOTA	398	0	VAL	63	9.608	20.583		1.00 27.24
	ATOM	399	N	SER	64	10.958	22.281	35.497	1.00 27.10
	ATOM	400	CA	SER	64	10.184	23.325	34.856	1.00 27.15
35	MOTA	401	CB	SER	64	9.714	24.383	35.860	1.00 27.28
	ATOM	402	OG	SER	64	10.732	25.312	36.206	1.00 27.39
•	ATOM	403	С	SER	64	11.205	23.919	33.889	1.00 27.74
•	ATOM	404	ō.	SER	64	12.408	23.908	34.156	1.00 28.32
	ATOM	405	Й	ILE	65	10.738	24.427	32.764	1.00 27.80
40	ATOM	406	CA	ILE	65	11.633	24.982	31.769	1.00 28.35
70				ILE	65	11.512	24.168	30.468	1.00 27.17
	MOTA	407	CB					29.419	1.00 26.25
	ATOM	408		ILE	65	12.444	24.709		1.00 20.23
	ATOM	409		ILE	65	11.812	22.695	30.773	
}	ATOM	410	-	ILE	65	11.570	21.747	29.611	1.00 27.91
′ 45 .	. ATOM	411	С	ILE .		11.282	26.446	31.538	1.00 29.42
	ATOM	412	0	ILE	65	10.243	26.767	30.968	1.00 29.87
	ATOM	413	. N	LYS	66	12.159	27.330	31.985	1.00 30.13
	ATOM	414	CA	LYS	66	11.925	28.755	31.861	1.00 31.66
	ATOM	415	CB	LYS	66	12.102	29.407	33.234	1.00 32.15
. 50	ATOM	416	CG	LYS	66	11.817	30.878	33.255	1.00 33.67
	ATOM .	417	CD	LYS	. 66	12.204	31.476	34.583	1.00 34.82
	MOTA	418	CE	LYS	66	11.748	32.922	34.672	1.00 36.66
	ATOM	419	NZ	LYS	66	12.031	33.530	36.011	1.00 38.73
					66	12.822	29.454	30.848	1.00 31.95
55	ATOM	420	C	LYS			29.331	30.905	1.00 31.33
55	ATOM	421	0	LYS	66	14.043			1.00 32.37
	MOTA	422	N ·	GLY	67	12.210	30.188		
	ATOM	423	CA	GLY	67	12.979	30.926	28.941	1.00 34.20
	MOTA	424	C	GLY	67	13.478	32.164	29.656	1.00 35.22
	MOTA	425	0	GLY .	67	12.688	33.018	30.037	1.00 36.31
60	ATOM	426	N	LAV	68	14.785	32.260	29.850	1.00 35.63
	MOTA	427	CA	VAL	68	15.375	33.383	30.561	1.00 37.07
	ATOM ·	428	CB	VAL	68	16.900	33.314	30.483	1.00 36.39

	7 move	429	CC1	VAL	68	17.509	34.445	31.278	1.00 35.24
	ATOM ATOM	430		VAL	68	17.371	31.969		1.00 36.82
	ATOM	431	C	VAL	68	14.928	34.780	30.121	1.00 38.09
	ATOM	431	0	VAL	68	14.363	35.537	30.121	1.00 38.43
5	ATOM	433	Ŋ	SER	69	15.179	35.133	28.870	1.00 38.89
9	ATOM	434	CA	SER	69	14.787	36.454	28.412	1.00 39.28
	ATOM	435	CB	SER	69	15.455	36.780	27.080	1.00 38.34
	MOTA	436	OG	SER	69	14.629	36.377	26.013	1.00 39.34
	ATOM	437	C	SER	69	13.270	36.616	28.293	1.00 39.46
10	ATOM	438	ŏ	SER	69	12.751	37.704	28.518	1.00 40.48
10	ATOM	439	N	ALA	70	12.555	35.551	27.952	1.00 39.48
	ATOM	440	CA	ALA	70 70	11.102	35.645	27.826	1.00 39.59
	ATOM	441	CB	ALA	70	10.565	34.441	27.064	1.00 39.12
	ATOM	442	C	ALA	70 70	10.436	35.724	29.190	1.00 39.70
15	ATOM	443	ŏ	ALA	70	9.306	36.191	29.320	1.00 40.04
10	ATOM	444	Ŋ	ASN	71	11.144	35.254	30.208	1.00 39.82
	ATOM	445	CA	ASN	71	10.633	35.246	31.567	1.00 39.73
	ATOM	446	СВ	ASN	71	10.442	36.683	32.077	1.00 39.99
	ATOM	447	CG	ASN	71	10.387	36.761	33.603	1.00 40.30
20	ATOM	448		ASN	71	11.195	36.140	34.287	1.00 40.54
	ATOM	449		ASN	71	9.441	37.531	34.135	1.00 39.59
	MOTA	450	C	ASN	71	9.314	34.477	31.629	1.00 39.75
	ATOM	451	ŏ	ASN	71	8.403	34.835	32:379	1.00 40.53
	ATOM	452	N	ARG	72	9.217	33.416	30.834	1.00 38.92
25	ATOM	453	CA	ARG	72	8.022	32.580	30.807	1.00 38.05
	ATOM	454	СВ	ARG	72	7.269	32.768	29.495	1.00 37.29
•	ATOM	455	CG	ARG	72	6.533	34.076	29.361	1.00 37.12
	ATOM	456	CD	ARG	72	6.058	34.238	27.921	1.00 37.64
	ATOM	457	NE	ARG	72	5.254	35.439	27.721	1.00 37.13
30	ATOM	458	CZ	ARG	72	. 3.935	35.495	27.863	1.00 36.23
	ATOM	459	NH1	ARG	72	3.245	34.419	28.201	1.00 35.39
	ATOM	460	NH2	ARG	72	. 3.308	36.641	27.674	1.00 36.87
	MOTA	461	С	ARG	72	8.395	31.105	30.958	1.0C 37.94
	* ATOM	462	0	ARG	72	9.508	30.697	30.625	1.00 37.86
35	ATOM	463	N	TYR	73	7.451	30.313	31.455	1.00 37.74
	ATOM	464	CA	TYR	7 3 .	7.652	28.883	31.655	1.00 36.75
	MOTA	465	CB	TYR	73	7.085	28.449	33.002	1.00 36.28
	MOTA	466	CG	TYR	73	7.695	29.181	34.149	1.00 35.96
	ATOM	467	CD1	TYR	73	7.225	30.438	34.529	1.00 36.06
40	ATOM	468	CE1	TYR	73	7.835	31.148	35.554	1.00 35.44
	ATOM	469	CD2	TYR	. 73	8.787	28.650	34.823	1.00 35.68
	ATOM	470	CE2	TYR	· 73	9.407	29.349	35.843	1.00 36.31
	ATOM	471	CZ	TYR	73	8.928	30.596	36.204	1.00 36.67
400	ATOM	472	OH	TYR	. 73	9.564	31.281	37.209	1.00 38.11
45	ATOM	473	C	TYR	73	6.972	28.067	30.572	1.00 36.72
	ATOM	474	0	TYR	73	5.833	28.337	30.198	1.00 37.00
	ATOM	475	N	LEU	74	7.666	27.054	30.080	1.00 36.29
	ATOM	476	CA	LEU	74	7.104	26.201	29.055	1.00 35.89
50	ATOM	477	CB	LEU	74	8.177	25.246	28.536	1.00 34.95
50 ·	ATOM	478	CG	LEU	74	7.730	24.233	27.488	1.00 33.69 1.00 34.02
	ATOM	479	CDI	LEU	74	7.607	24.944	26.150 27.408	1.00 34.02
	MOTA	480		LEU	74	8.731 5.949	23.095	29.652	1.00 35.30
	MOTA	481	C	TEO	74 74	6.042	25.406 24.907	30.776	1.00 35.25
55	MOTA	.482	0	LEU		4.862	24.907	28.895	1.00 35.45
J)	ATOM	483	N	ALA	75 75	3.691		29.344	1.00 37.11
	ATOM	484	CA	ALA	75 75		24.545 25.491	29.344	1.00 38.41
	ATOM	485	CB	ALA	75 75	2.660 ·	23.491	28.170	1.00 37.93
	ATOM	486	C	ALA ALA	75 75 .	3.084	24.323	27.048	1.00 39.32
60	MOTA	487	O N	MET	75 . 76 ·	2.530	22.629	28.427	1.00 39.83
UU.	ATOM ATOM	488	N CA		76 76	1.860	22.629	27.386	1.00 40.20
		489 490	CA CB	MET MET	76	2.420	20.438	27.279	1.00 41.81
	ATOM	43 J U	CD	LILL	70	2.420	20.430	21.213	1.00 41.01

	ATOM	491	CG	MET	76	1.754	19.646	26.172	1.00 41.84
	ATOM	492		MET	76	2.515	18.069	25.840	1.00 45.00
•			SD						
	ATOM	493	.CE	MET	76	1.593	17.044	26.896	1.00 44.29
	ATOM	494	С	MET	76	0.382	21.786	27.743	1.00 42.49
5.	ATOM	495	0	MET	76	0.024	21.447	28.872	1.00 41.69
_									
	ATOM	496	N	LYS	77	-0.475	22.093	26.775	1.00 43.54
	ATOM	497	CA	LYS	77	-1.906	22.106	27.019	1.00 44.58
	ATOM	498	CB	LYS	77	-2.553	23.140	26.113	1.00 44.50
	MOTA	499	CG	LYS	77	-1.814	24.457	26.102	1.00 45.41
10	MOTA	500	CD	LYS	77	-2.451	25.481	27.027	1.00 46.70
	ATOM	501	CE	LYS	77	-2.364	25.068	28.474	1.00 46.80
					7 7	-2.880	26.148	29.356	
	ATOM	502	NZ	LYS					1.00 47.00
	ATOM	503	С	LYS	77 ·	-2.585	20.755	26.842	1.00 44.85
	ATOM	504	0	LYS	77	-1.953	19.778	26.443	1.00 44.74
15	ATOM	505	N	GLU	78	-3.880	20.728	27.146	1.00 45.05
13									
	MOTA	506	CA	GT U	78	-4.711	19.537	27.057	1.00 45.21
	ATOM	507	CB	GLU	78 ·	-6.124	19.865	27.531	1.00 44.54
	ATOM	508	CG	GLU	78	-6.904	20.817	26.625	1.00 44.11
	MOTA	509	CD	GLU	78	-6.328	22.231	26.562	1.00 44.45
20	ATOM	510	OE1	GLU	78	-5.909	22.770	27.615	1.00 43.37
	MOTA	511	OE2	GLU	78	-6.316	22.815	25.453	1.00 44.41
}	MOTA	512	С	GLU	. 78	-4.787	18.964	25.647	1.00 45.90
	ATOM	513	0	GLU	78	-4.994	17.760	25.465	1.00 46.07
	MOTA	514	N	ASP	79	-4.642	19.828	24.647	1.00 45.95
2:5		515			79		19.382	23.256	
23	MOTA		CA	ASP		-4.695			1.00 45.54
	ATOM	516	СB	ASP	79	-5.215	20.495	22.342	1.00 45.86
	MOTA	517	CG	ASP	79	4.272	21.680	22.279	1.00 47.04
	ATOM	518		ASP	79	-4.444	22.551	21.398	1.00 47.93
•									
	MOTA	519		ASP	79	-3.354	21.748	23.120	1.00 47.75
30	ATOM	520	С	ASP	79	-3.317	18.956	22.771	1.00 44.86
	ATOM	521	0	ASP	79	-3.184	18.346	21.711	1.00 45.40
		522							
	MOTA		. N	GLY	80 .	-2.291	·19.288	23.543	1.00 43.77
,	ATOM	523	CA	GLY	8C '	-0.942	18.922	23.166	1.00 42,64
•	MOTA	524	С	GLY	. 80	- :0.095	20.066	22.639	1.00 42.17
35	ATOM	525	Ö	GLY	80	1.094	19.885	22.374	1.00 41.86
55									1.00 41.00
	ATOM	526	N	ARG	81 .	-0.683	21.248	22.483	1.00 41.13
	ATOM	527	CA	ARG	81	.0.083	22.373	21.970	1.00 40.34
	ATOM	528	CB	ARG	81	-0.845	23.457	21.409	1.00 39.97
40	MOTA	529	CG		. 81	-1.616	24.242	22.436	1.00 39.13
40	MOTA	530	CD	ARG	81	-2.404	25.358	21.781	1.00 38.12
	ATOM	531	NE	ARG	81	-3.042	26.185	22.795	1.00 38.02
	ATOM	532	CZ	ARG	81	-3.965	25.734	23.639	1.00 38.95
								-	
	ATOM	533	NH1		81	-4.361	24.464	23.580	1.00 38.84
	MOTA	534	· NH2	ARG	81	-4.481	26.546	24.553	1.00 38.18
45	ATOM	535	С	ARG	81 ·	0.995	22.950	23.046	1.00 39.91
	ATOM	536	ŏ	ARG	81	0.751	22.765	24.242	1.00 40.38
	MOTA	537	N	LEU	82	2.056	23.631	22.616	1.00 38.75
	ATOM	538	CA	LEU	82	3.022	24.222	23.540	1.00 37.93
	ATOM	539	СВ	LEU	82	4.456	23.802	23.171	1.00 36.21
50									
50	ATOM	540	CG	LEU	82	4.829	22.315	23.052	1.00 34.01
	ATOM	541	CD1	LEU	82	6,329	22.173	22.841	1.00 32.17
	ATOM	542	CD2	LEU	82	4.406	21.582	24.304	1.00 32.98
					02				
	ATOM	543	С	LEU	82	2.962	25.740	23.566	1.00 38.10
	MOTA	544	0	LEU	82	2.668	26.383	22.559	1.00 38.60
55 '	ATOM	545	N	LEU	83	3.246	26.314	24.724	1.00 38.19
	ATOM	546	CA	LEU	83	3.254	27.763	24.862	1.00 38.46
	MOTA	547	CB	LEU	83	1.826	28.314	24.901	1.00 37.52
	ATOM	548	CG	LEU	83	0.862	27.819	25.981	1.00 37.54
	ATOM	549			83	1.342	28.260		
60									1.00 36.95
60	ATOM	550	CD2		83	÷0.537	28.369	25.696	1.00° 36.58
	ATOM	551	С	LEU	83	. 4.009	28.118	26.129	1.00 38.76
	ATOM	552	ō	LEU	83	4.258	27.252	26.967	1.00 39.02
	*** 051	JJ2	_		ري	3.200	21.232	20.301	2.00 33.02

		•							
	ATOM	553	N	ALA	84	4.385	29.383	26.265	1.00 39.18
	ATOM	554	CA	ALA	84	5.120	29.813	27.445	1.00 40.26
	ATOM	555	CB	ALA	84	6.376	30.565	27.037	1.00 40.39
	ATOM	556	C	ALA	84	4.256	30.682	28.347	1.00 40.54
5	ATOM	557	Ō	ALA	84	3.981	31.837	28.034	1.00 40.58
_	ATOM ·	558	N	SER	85	3.832	30.122	29.477	1.00 40.83
	ATOM	559	CA	SER	85	2.995	30.872	30.393	1.00 40.42
	ATOM	560	CB	SER	85	2.084	29.944	31.207	1.00 39.27
	ATOM	561	OG	SER	85	2.701	29.482	32.387	1.00 39.17
10		562		SER ·		3.824	31.763	31.302	1.00 41.15
10	ATOM	563	C	SER	85	4.985	31.478	31.598	1.00 41.13
	ATOM				86	3.219	32.867	31.721	1.00 41.83
•	ATOM	564	N	LYS		3.889			1.00 41.83
	ATOM	565	CA	LYS	86		33.831	32.582	
1.5	MOTA	566	CB	LYS	86	3.161	35.179	32.549	1.00 42.91
15	MOTA	567	CG	LYS	86	4.079	36.405	32.586	1.00 43.72
	MOTA	568	CD	LYS	86	4.949	36.496	31.320	1.00 44.37
	MOTA	569	CE	LYS	86	5.702	37.838	31.197	1.00 43.85
	MOTA	570	NZ	LYS	86	6.653	38.119	32.319	1.00 43.40
	ATOM	571	С	LYS	86	3.958	33.326	34.012	1.00 42.58
20	ATOM	572	0	LYS	86	4.888	33.664	34.742	1.00 43.32
	MOTA	573	N	SER	87	2.978	32.529	. 34.423	1,00 42.41
	ATOM	574	CA	SER	87	2.990	31.985	35.780	1.00 42.99
	MOTA	575	CB	SER	87	1.769	32.459	36.578	1.00 43.28
	MOTA	576	OG	SER	87	0.566	32.014	35.988	1.00 45.27
25	MOTA	577	С	SER	87	3.054	30.459	35.757	1.00 42.54
	ATOM	578	0	SER	87	2.723	29.826	34.760	1.00 42.59
	ATOM	579	N	VAL	88	3.479	29.876	36.868	1.00 42.19
	ATOM	580	CA	VAL	88	3.631	28.431	36.961	1.00 42.00
	ATOM	581	СВ	VAL	88	4.668	28.057	38.043	1.00 41.45
30.	ATOM	582	CG1		88	4.908	26.555	38.039	1.00 41.94
	ATOM	583	CG2		88	5.952	28.804	37.802	1.00 40.44
•	ATOM	584	c	VAL	88.	2.346	27.693:		1.06 41.90
	ATOM .	585	ŏ	VAL	88	1.694	27.967	38.265	1.00 41.91
	ATOM	586	Ñ	THR	89	2.001	26.737	36.419	1.00 42.31
35	ATOM	587	CA	THR	89	0.7.99	25.929	36.602	1.00 43.07
55	ATOM	588	CB	THR	89	-0.196	26.129	35.470	1.00 42.64
	ATOM	589	OG1		89	0.337	25.540	34.279	1.00 40.99
	ATOM	590	CG2		89	-0.460	27.613	35.247	1.00 42.22
	MOTA	591	C	THR	89	1.218	24.470	36.551	1.00 43.77
40	MOTA	592	ŏ	THR	89	2.358	24.165	36.214	1.00 44.96
-10	ATOM	593	N	ASP	90 .	0.297	23.564	36.856	1.00 43.62
	ATOM	594	CA	ASP	90	0.612	22.142	36.836	1.00 43.36
	ATOM	595	CB	ASP	90	-0.571	21.337	37.382	1.00 44.19
	ATOM	596	CG	ASP	90	-1.848	21.546	36.571	1.00 46.79
45	ATOM	597		ASP	90	-1.899	22.500	35.756	1.00 47.51
43		598		ASP	90	-2.809	20.760	36.758	1.00 48.03
	ATOM .				· 90	0.975	21.649	35.437	1.00 42.81
	MOTA	. 599	C	ASP ASP	90	1.440		35.273	1.00 42.81
	ATOM	600	0			0.766		34.424	1.00 43.00
50	ATOM	· 601	N	GLU	91		22.483		
50	ATOM	602	CA	GLU	. 91	1.091	22.086	33.054	1.00 40.04
	ATOM	603	CB	GLU	91	0.076	22.672	32.069	1.00 39.51
	MOTA	604	CG	GLU	91	-1.329	22.109	32.215	1.00 39.37
	MOTA	605	CD	GLU	91	-2.313	22.698	31.208	1.00 39.86
	ATOM .	606		GLU	91	-2.338	23.935	31.041	1.00 40.41
55	MOTA	607		GLU	91	-3.072	21.929	30.590	1.00 39.43
	ATOM .	608	С	GLU	91	2.496	22.527	32.659	1.00 38.71
	ATOM	609	0	GLU	91	2.880	22.438	31.495	1.00 38.40
	ATOM	61 Q	N	CYS	92	3.261	22.995	33.638	1.00 36.91
	ATOM	611	CA	CYS	92	4.614	23.469	33.384	1.00 35.73
60	ATOM	612	·CB	CYS	92	4.811	24.838	34.036	1.00 35.48
	ATOM	613	SG	CYS	92	3.619	26.089	33.511	1.00 33.42
	ATOM	614	C	CYS	92	5.693	22.519	33.886	1.00 34.96

	•								
	ATOM	615	0	CYS	92	6.876	22.863	33.873	1.00 34.46
	ATOM	616	N	PHE	93	5.288	21.328	34.323	1.00 34.01
	MOTA	617	CA	PHE	93	6.241	20.357	34.847	1.00 33.41
_	MOTA	618	CB	PHE	93	5.841	19.973	36.274	1.00 33.36
5	ATOM	619	CG	PHE	. 93	5.797	21.147	37.217	1.00 33.71
	ATOM	620	CD1		93	6.973	21.800	37.593	1.00 34.28
	ATOM	621	CD2		93	4.582	21.634	37.694	1.00 33.99
	ATOM	622	CE1		93	6.941	22.928	38.431	1.00 33.93
	ATOM	623	CE2		93	4.537	22.757	38.529	1.00 33.44
10	ATOM	624	CZ	PHE	93	5.720	23.404	38.896	1.00 33.83
	ATOM	625	C	PHE .	93	6.394	19.122	33.968	1.00 32.60
	MOTA	626	0	PHE	93	5.410	18.565 18.710	33.470 33.779	1.00 32.56 1.00 31.35
	MOTA	627	N	PHE	94 94	7.644 7.956	17.570	32.933	1.00 31.33
15	ATOM	628	CA	PHE	94	8.574	18.053	31.630	1.00 30.20
13	ATOM	629	CB	PHE	94	7.761	19.088	30.936	1.00 28.30
	MOTA MOTA	630 631	CG CD1	PHE	94	6.778	18.717	30.020	1.00 27.94
	ATOM	632	CD2		94	7.917	20.432	31.254	1.00 26.64
	ATOM	633	CE1		94	5.961	19.674	29.440	1.00 28.07
20	ATOM	634	CE2		94	7.107	21.388	30.683	1.00 26.92
20	ATOM	635	CZ	PHE	94	6.125	21.014	29.775	1.00 26.80
	ATOM	636.		PHE	94	8.930	16.624	33.585	1.00 30.36
	ATOM	637	ŏ	PHE	94	9.768	17.041	34.387	1.00 30.51
	ATOM		. N	PHE	95	8.815	15.344	33.242	1.00 30.11
25	ATOM .		CA	PHE	95 ·	9.736	14.345	33.757	1.00 29.83
	MOTA	640	CB	PHE	95	9.161	12.933	33.663	1.00 30.35
	ATOM	641	CG	PHE	95	7.882	12.735	34.417	1.00 31.10
	MOTA	642	CD1	PHE	95	6.679	12.586	33.733	1.00 31.54
	MOTA	643	CD2	PHE	.95	7.876	12.690	35.807	1.00 30.85
. 30	MOTA	644		PHE	95 .	5.488	12.394	34.422	1.00 32.11
	MOTA	645	CE2		95	6.692	12.499	36.508	1.00 31.21
•	MOTA	646	CZ	PHE	95	5.493	12.351	35.815	1.00 31.97
	MOTA	647	С	PHE	95	10.933	14.432		1.00 29.77
25	ATOM	648	0	PHE	95	10.807	14.231	31.616	1.00 30.05
. 35	ATOM	649	N.	GLU	96 06	12.087	14.763	33.384	1.00 29.61 1.00 29.17
	ATOM	650	CA	GLU -	96 96	13.301 14.217	14.856 15.960	32.599 33.131	1.00 29.17
•	ATOM	651	CB	GLU	96	15.555	16.033	32.401	1.00 28.32
	ATOM . ATOM	652 653	CG	GLU		16.507	17.072	32.972	1.00 28.28
· 40	ATOM	654	OE1		96 . 96	16.830	17.003	34.176	1.00 28.47
40	ATOM	655	OE2	GLU	96	16.949	17.957	32.213	1.00 29.85
	ATOM	656	c	GLU	96	14.019	13.524 -		1.00 29.36
	ATOM	657	ŏ	GLU	96	14.392	13,097	33.791	1.00 29.94
	ATOM	658	N	ARG	97	14.211	12.865	31.568	1.00 29.12
45	ATOM	659	CA	ARG	97	14.899	11.589	31.569	1.00 28.94
	ATOM	660	CB	ARG	97	13.942	10.464	31.176	1.00 30.10
	ATOM	661	CG	ARG	97	14.557	9.084	31.295	1.00 32.11
	ATOM	662	CD	ARG	97	13.709	8.004	30.615	1.00 34.80
	ATOM	663	NE	ARG	97	14.268	6.657	30.783	1.00 36.88
50	ATOM	664	CZ	ARG	97	14.296	5.988	31.939	1.00 38.16
	ATOM	665		ARG	97	.13.795	6.528	33.046	1.00 38.69
	ATOM	666	NH2		97	14.829	4.774	31.992	1.00 39.07
	ATOM	667	С	ARG	97	16.100	11.551	30.636	1.00 27.85
	ATOM	668	0	ARG	97	16.029	11.979	29.489	1.00 27.26
55 .	MOTA	669	N	LEU	98	17.209	11.052	31.162	1.00 26.65
	ATOM	670	CA	LEU	98	18.417	10.890	30.388	1.00 26.16
	ATOM	671	CB	LEU	. 98	19.662	10.983	31.283	1.00 25.10
	ATOM	672	CG	TEO	98	20.922	10.397	30.639	1.00 23.67
60	ATOM	673		LEU	. 98	21.103	10.977	29.239 31.520	1.00 22.19
60	ATOM	674		LEU	98	22.124	10.663 9.478	29.837	1.00 23.41 1.00 26.51
	MOTA	675 676	C	LEU	98 98	18.256 18.473	9.478 8.488	30.537	1.00 26.31
	ATOM	0/0	U	LEU	20	10.4/3	0.400	JU.JJ/	**** EA**

	ATOM	677	N .	GLU	99	17.848	9.393	28.581	1.00 26.80
	ATOM	678	CA	GLU	99	17.622	8.115	27.936	1.00 26.82
				GLU	99	16.927	8.348	26.603	1.00 26.24
	MOTA	679	CB						
	MOTA	680	CG	GLU	99	15.639	9.147	26.718	1.00 28.42
· 5	ATOM	681	CD	GLU	99	14.450	8.315	27.191	1.00 28.95
٠.			OE1	GLU	99	13.337	8.879	27.350	1.00 28.29
•	MOTA	682							
	MOTA	683	OE2	GLU	99	14.627	7.096	27.399	1.00 30.66
	ATOM	684	С	GLU	99	18.915	7.341	27.719	1.00 27.08
								27.759	1.00 27.12
	ATOM	685	0	GLU	99	20.008	7.902		
10	ATOM	686	N	SER	100	18.775	6.048	27.469	1.00 27.05
	ATOM	687	CA	SER	100	19.921	5.192	27.247	1.00 27.22
	· ATOM	688	CB	SER	100	19.476	3.744	27.150	1.00 28.27
	MOTA	689	OG	SER	· 100	18.748	3.559	25.957	1.00 31.47
		690		SER	100	20.697	5.565	25.993	1.00 26.70
	MOTA		C						
15	MOTA	691	0	SER	100	21.835	5.147	25.830	1.00 26.34
	ATOM	692	N	ASN	101	20.093	6.337	25.096	1.00 26.70
				ASN	101	20.813	6.746	23.886	1.00 25.33
	MOTA	693	CA						
	ATOM	694	CB	asn	101	19.866	6.891	22.709	1.00 25.22
	ATOM	695	CG	ASN	101	19.005	8.107	22.826	1.00 26.50
20							8.668	23.916	1.00 26.62
20	ATOM	696	OD1	ASN	101	18.848			
	MOTA	697	ND2	ASN	101	. 18.426	8.529	21.709	1.00 27.53
`\	ATOM	698	C	ASN	101	21.540	8.071	24.108	1.00 24.54
)									
	MOTA	699	0	ASN	101	22.061	8.662	23.:175	1.00 24.37
	ATOM	700	N	ASN	102	21.566	8.514	25.361	1.00 24.45
25	ATOM	701	CA	ASN	102	22.213	9.755	25.808	1.00 24.46
23									
	MOTA	702	CB	ASN	102	23.698	9.785	25.450	1.00 23.96
	MOTA	703·	CG	ASN	102	24.512	8.820	26.292	1.00 25.70
				ASN	102	24.287	8.676	27.493	1.00 26.34
	MOTA	704							
	ATOM	705	ND2	ASN	102	25.467	8.151	25.663	1.00 27.30
30	MOTA	706	С	ASN	102	21.566	11.073	25.432	1.00 24.22
-					102	22.197	12.122	25.470	1.00 24.68
	MOTA	707	0	ASN					
	MOTA	708	N	ŢYR	103	20.297	·11.018	25.077	1.00 24.01
	MOTA	709	CA	TYR	103	19.561	12.229	24.788	1.00 24.03
							12.112	23.443	1.00 23.95
	MOTA	710	CB	TYR	103	18.867			
35	· ATOM	711	CG	TYR	103	19.776	12.339	22.254	1.00 24.32
	ATOM	712	CD1	TYR	103.	19.955	13.621	21.722	1.00 22.76
								20.584	1.00 23.37
	MOTA	713	CE1	TYR	103	20.710	13.822		
	ATOM	714	CD2	TYR	103	20.395	11.262	21.615	1.00 23.85
	ATOM	715	CE2		103	21.158	11.454	20.465	1.00 24.34
40									
40	ATOM	716	CZ	TYR	103	21.304	12.734	19.956	1.00 24.60
	MOTA	717	OH	TYR	103	22.012	12.908	18.794	1.00 27.78
	ATOM	718	C	TYR	103	18.539	12.346	25.924	1.00 24.04
				•					
	MOTA	719	. 0	TYR	103	18.246	11.367	26.612	1.00 23.70
` \	MOTA	720	N	ASN	104	18.026	13.545	26.149	1.00 24.29
¹ 45	ATOM	721	CA	ASN	104	17.036	13.752	27.192	1.00 24.08
~ 43									
	MOTA	722	CB	ASN	104	17.300	15.056	27.923	1.00 24.06
	MOTA	723	CG	ASN	104	18.481	14.977	28.858	1.00 24.66
					104	19.305	14.056	28.785	1.00 23.53
	ATOM	724		ASN					
	MOTA	725	ND2	ASN	104	18.580	15.961	29.745	1.00 24.15
50	ATOM	726	C	ASN	104	15.662	13.828	26.570	1.00 24.42
30							14.204	25.410	1.00 24.35
	ATOM	727	0	ASN	104	15.516			1.00 24.33
	MOTA	728	N	THR	105	14.653	13.438	27.334	1.00 25.04
		729	CA	THR	105	13.268	13.530	26.887	1.00 25.02
	ATOM								
	MOTA	730	CB	THR	105	12.552	12.147	26.727	1.00 24.65
55	ATOM	731	OG1	THR	105	12.721	11.354	27.909	1.00 24.73
55		722				13.069	11.406	25.510	1.00 23.90
	ATOM	732	CG2		105				
	MOTA ·	733	С	THR	105	12.557	14.313	27.973	1.00 25.71
	MOTA	734	0	THR	105	13.003	14.350	29.113	1.00 25.75
							14.955	27.613	1.00 26.81
	ATOM	735	N	TYR	106	11.462			
60	MOTA	736	CA	TYR	106	10.694	15.730	28.570	1.00 27.94
	ATOM	737	CB	TYR	106	10.933	17.211	28.330	1.00 27.66
									1.00 27.77
	ATOM	738	CG	TYR	106	12.350	17.580	28.653	1.00 27.77

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CD1 TYR
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                                             12.738
                                                      17.805
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          ATOM
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          ATOM
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                                                               30.276
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	ATOM	807	C	SER	113		2.557	11.049	26.374	1.00 35.98
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	ATOM	808	0	SER	113					
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10	ATOM	810	CA	TRP	114		3.020	13.283	25.601	1.00 35.24
	MOTA	811	CB	TRP	114		1.953	14.364	25.422	1.00 36.67
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	ATOM	812	CG	TRP	114					
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	ATOM .	814	CE2	TRP	114		-1.650	13.665	24.657	1.00 40.04
15	MOTA	815	CE3	TRP	114		-1.010	15.817	25.567	1.00 39.40
				TRP	114		0.306	12.592	24.564	1.00 38.75
	ATOM	816						-		
	ATOM	817	NE1	TRP	114		-1.043	12.486	24.313	1.00 39.11
	ATOM	818	CZ2	TRP	114	-	-2.997	14.043	24.584	1.00 40.56
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20	ATOM	820	CH2		114		-3.320	15.306	25.007	1.00 40.55
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	MOTA	822	0	TRP	114			14.245	27.071	1.00 33.96
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25							7.580	13.750	24.385	1.00 30.98
25	ATOM	825	СВ	TYR	115					
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	ATOM	827	CD1	TYR	115		6.887	11.347	24.616	1.00 29.82
	MOTA	828	CE1	TYR '	115		7.071	10.075	25.113	1.00 31.32
	ATOM	829	CD2	TYR	115		8.784	12.111	25.862	1.00 30.94
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	· ATOM	831	CZ	TYR	115		8.123	9.824	25.994	1.00 31.82
•	MOTA	832	OH-	TYR	115	•	8.313	8.559	26.494	1.00 32.48
	ATOM	933	C	TYR	115		6.671	16.000	24.379	1.00 30.22
•								16.328	23.433	1.00 30.13
	ATOM	834	Ο.	TYR	115		5.950			
35	MOTA	. 83 5	N	VAL	116		7.623	16.775	24.886	1.00 29.29
	ATOM	836	CA	VAL	116		7.936	18.072	24.315	.1.00 29.10
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		838		VAL	116		9.291	20.164	24.578	1.00 26.24
	ATOM	839	CG2		116		8.248	19.066	26.585	1.00 26.68
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	ATOM	846	0	ALA	117		8.065	19.890	19.599	1.00 32.32
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50	ATOM	850	CG	LEU	118		11.348	21.637	18.897	1.00 33.25
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                                                       18.771
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                                              -1.426
          MOTA
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                                                       20.404
                                                                18.784
                                                                         1.00 36.46
                                    126
                                              -0.683
                   921
                        CD2 LEU
          MOTA
                                                                         1.00 40.33
    60
                                                       17.278
                                                                20.053
                                               2.172
          MOTA
                   922
                        С
                             LEU
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                                             2.511
                                                       16.212
                                                                19.538
                                                                         1.00 40.56
                   923
                             LEU
                                    126
          ATOM
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                                               2,093
                                                       17.449
                                                                21.366
                                                                         1.00 40.46
          MOTA
                   924
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		MOTA	925	CA	GLX	127	2.404	16.353	22.264	1.00 40.66
		ATOM	926	С	GLY	127	1.529	15.149	21.978	1.00 40.63
		ATOM	927	0	GLY	127	1.954	14.009	22.125	1.00 39.82
		ATOM	928	N	SER	128	0.298	15.413	21.555	1.00 40.87
	5	ATOM	929	CA	SER	128	-0.651	14.358	21.250	1.00 41.21
•	•	ATOM	930	CB.	SER	128	-1.991	14.975	20.900	1.00 40.69
			931		SER	128	-1.812	15.943	19.890	1.00 40.89
		MOTA		OG						
		ATOM	932	. C	SER	128	-0.173	13.501	20.090	1.00 41.64
	10	ATOM	933	0	SER	128	-0.647	12.391	19.890	1.00 40.99
	10	MOTA	934	N	LYS	129	0.772	14.024	19.321	1.00 42.40
		MOTA	935	CA	LYS	129	1.295	13.288	18.186	1.00 42.92
		MOTA	936	CB	LYS	129	1.267	14.180	16.942	1.00 43.84
		MOTA	937	CG	LYS	129	-0.141	14.329	16.387	1.00 45.32
		ATOM .	938	CD	LYS	129	-0.260	15.387	15.307	1.00 47.16
	15	ATOM	939	CE	LYS	129	-1.710	15.461	14.812	1.00 48.88
		MOTA	940	NZ	LYS	129	-1.985	16.588	13.866	1.00 50.31
		ATOM	941	C	LYS	129	2.690	12.719	18.426	1.00 42.38
		ATOM	942	ŏ	LYS	129	3.289	12.142	17.528	1.00 42.01
		ATOM	943	N	THR	130	3.194	12.860	19.649	1.00 42.01
	<u>2</u> 0	MOTA	944	CA	THR	130	4.523	12.354	19.983	1.00 41.66
•	20					130	5.192			
`\		ATOM	945	CB	THR			13.176	21.106	1.00 40.68
)		ATOM	946		THR	130	4.489	12.962	22.334	1.00 39.45
		ATOM	947		THR	130	5.195	14.662	20.760	1.00 40.36
	25	ATOM	948	C	THR	130	. 4.479	10.903	20.443	1.00 41.78
•	25	ATOM	949	0	THR	130	3.413	10.361	20.724	1.00 41.50
		MOTA		N	GLY	131	5.655	10.286	20.518	1.00 42.00
		MOTA	951	CA	GLY	131	. 5.758	8.904	20.946	1.00 41.91
		MOTA	952	С	GLY	131	7.195	8.581	21.290	1.00 42.14
		MOTA	953	0	GLY	131	8.095	9.317	20.895	1.00 42.22
	30	ATOM	954	N	PRO	132	7.446	7.474	22.007	1.00 42.30
		MOTA	955	CD	PRO	132	6.418	6.505	22.417	1.00 41.73
		ATOM	956	CA	PRO	132	8.773	7.015	22.433	1.00 42.12
•	٠.	ATOM	957	СВ	PRO	132	8.472	5.689	23.133	1.00 41.91
		ATOM	958	CG	2RO	132	7.076	5.843	23.593	1.00 42.30
:	35	ATOM	959	C	PRO	132	9.775	6.813	21.300	1.00 42.01
		ATOM	960	ō	PRO	132	10.964	7.125	21.433	1.00 43.09
		ATOM	961	N	GLY	133	9.296	6.273	20.188	1.00 41.52
		ATOM	962	CA	GLY	133	10.188	6.016	19.074	1.00 41.10
		ATOM	963	C	GLY	133	10.383	7.152	18.093	1.00 40.19
	40	ATOM	964	ŏ	GLY	133	10.687	6.910	16.931	1.00 40.19
		ATOM	965	N	GTN .	134	. 10.227	8.391	18.544	1.00 39.31
		ATOM .	966	CA	GLN	134	. 10.400	9.518	17.641	1.00 39.31
						134				
٠.		ATOM	967	CB	GLN.	134	9.198	10.446	17.702	1.00 37.90
, j	45·	ATOM	968	CG	GLN		7.906	9.770	17.364	1.00 37.73
•	+2.	ATOM	969	CD	GLN	134	6.746	10.728	17.356	1.00 37.43
_		ATOM	970	OE1		134	5.592	10.318	17.272	1.00 37.42
		ATOM	971	NE2		134 .	7.044	12.016	17.435	1.00 37.10
		MOTA	972	С	GLN	134	11.654	10.323	17.910	1.00 37.85
		ATOM	973	. 0	GLN	134	12.078	10.497	19.052	1.00 38.47
	50	ATOM	974	N	LYS	135	12.236	10.822	16.833	1.00 36.65
-		ATOM	975	CA	LYS	135	13.443	11.623	16.883	1.00 35.45
	•	ATOM	.976	CB	LYS	135	14.025	11.660	15.475	1.00 35.04
		ATOM	977	CG	LYS	135	15.316	12.391	15.261	1.00 36.23
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:	55	ATOM	979	CE	LYS	135	16.943	12.925	13.375	1.00 37.17
		ATOM	980	NZ	LYS	135	17.400	12.513	12.026	1.00 37.53
		ATOM	981	·C	LYS	135	13.126	13.031	17.388	1.00 37.33
		ATOM	982	0		135	13.120	13.722		
					LYS				17.929	1.00 35.38
	б0 ·	ATOM '	983	N	ALA	136	11.868	13.435	17.235	1.00 33.78
•	UU	ATOM	984	CA	ALA	136	11.413	14.764	17.631	1.00 32.23
		ATOM	985	CB	ALA	136	10.042	15.022	17.051	1.00 31.71
		MOTA	986	С	ALA	136	11.385	15.041	19.126	1.00 31.58

		ATOM	987	0	ALA	136	11.396	16.198	19.538	1.00 31.40
		ATOM	988	N	ILE	137	11.359	13.988	19.935	1.00 30.43
		ATOM	989	CA	ILE	137	11.299	14.136	21.383	1.00 29.08
	_	ATOM	990	CB	ILE	137	10.505	12.971	22.010	1.00 28.62
	5	ATOM	991	CG2		137	9.097	12.878	21.396 21.786	1.00 27.72 1.00 27.64
		ATOM	992	CG1		137	11.263	11.660	22.574	1.00 27.84
		MOTA	993	CD1		137	10,712	10.490 14.167	22.063	1.00 20.05
		MOTA	994	C	ILE	137 137	12.663 12.760	14.447	23.255	1.00 29.51
	10	ATOM	995 996	0	LEU	137	13.714	13.884	21.306	1.00 28.48
	10	ATOM	996	N CA	TEA	138	15.067	13.822	21.855	1.00 27,74
		ATOM ATOM	998	CB	LEU	138	15.866	12.767	21.081	1.00 25.88
			999	CG	LEU	138	15.234	11.370	21.120	1.00 23.44
		ATOM	1000	CD1		138	15.866	10.470	20.079	1.00 23.09
	15	ATOM	1001	CD2		138	15.406	10.782	22.512	1.00 21.50
		ATOM	1002	C	LEU	138	15.822	15.143	21.871	1.00 27.94
		ATOM	1003	Ō	LEU	138	15.954	15.810	20.849	1.00 29.08
		ATOM	1004	N	PHE	139	16.327	15.516	23.038	1.00 27.46
		ATOM	1005	CA	PHE	139	17.058	16.765	23.158	1.00 27.29
	20 .	MOTA	1006	CB	PHE	139	16.253	17.778	23.973	1.00 26.26
		MOTA	1007	CG	PHE	139	14.982	18.221	23.313	1.00 24.21
}		MOTA	1008		PHE	139	13.839	17.441	23.387	1.00 23.67
•		MOTA	1009		PHE	139	14.922	19.441	22.644	1.00 23.89
		ATOM	1010		PHE	139	12.650	17.871	22.810	1.00 23.55
	25	MOTA	1011	-	PHE	139	13.741	19.884	22.062	1.00 23.26
		MOTA	1012	CZ	PHE	139	12.602	19.100	22.146	1.00 23.71
		MOTA	1013	C	PHE	139	18.411	16.588	23.805 24.720	1.00 27.66 1.00 27.66
		ATOM	1014	0	PHE	139	18.578 19.380	15.796 17.345	23.320	1.00 27.00
	30	ATOM	1015	N	LEU	140 140	20.718	17.291	23.864	1.00 29.25
	<i>3</i> 0	ATOM ATOM	1016 1017	CA CB	LEU	140	21.738	17.164	22.739	1.00 27.95
		ATOM	1017	CG.	LEU	140	23.173	16.905	23.167	1.00 27.42
•		MOTA	1019		LEU	140	23.232	15.557	23.885	1.00 27.33
		ATOM	1020		LEU	140	24.112	16.930	21.989	1.00 27.78
	35	ATOM	1021	C	LEU	140	20.960	18.584	24.628	1.00 30.43
	•	ATOM	1022	0	LEU	140 -	21.002	19.662	24.036	1.00 31.10
		ATOM	1023	N	PRO	141	21.080	18.505	25.959	1.00 30.89
		ATOM	1024	CD	PRO	141	20.724	17.391	26.850	1.00 30.79
		ATOM	1025	CA	PRO	141 .		19.725	26.725	1.00 32.44
	40	ATOM	1026	CB	PRO	141	21.023	19.305	28.166	1.00 31.35
		MOTA	1027	CG	PRO	141	21.308	17.839	28.164	1.00 31.22
		ATOM	1028	Ċ	PRO	141	22.747	20.230	26.536	1.00 34.14
		ATOM	1029	0	PRO	141	23.707	19.464	26.572	1.00 34.05 1.00 36.45
}	45	MOTA	1030	N	MET	142	22.872	21.529	26.320 26.110	1.00 38.91
	45	MOTA	1031	CA	MET MET	142 142	24.166 24.315	22.148 22.519	24.640	1.00 37.58
		MOTA	1032	CB CG	MET	142	24.203	21.341	23.701	1.00 36.89
		MOTA MOTA	1033 1034	SD	MET .	142	24.345	21.837	21.984	1.00 37.07
		ATOM	1034	CE	MET	142	26.022	22.298	21.902	1.00 37.42
	50 .		1035	C	MET	142	24.244		26.964	
	J U .	ATOM ATOM	1037	ŏ	MET	142	23.239	24.079	27.152	1.00 41.83
		ATOM	1038	N	SER	143	25.426	23.696	27.487	1.00 44.37
		ATOM	1039	CA	SER	143	25.576	24.883	28.313	1.00 47.76
		ATOM	1040	CB	SER	143	26.992	24.980	28.876	1.00 48.30.
	55	ATOM	1041	OG	SER	143	27.921	25.277	27.848	1.00 49.63
		ATOM	1042	Ċ	SER	143	25.282	26.106	27.457	1.00 49.81
		ATOM	1043	.0	SER	143	25.415	26.071	26.228	1.00 50.18
		ATOM	1044	N	ALA	144	24.866	27.184	28.105	1.00 52.23
		MOTA	1,045	CA	ALA	144	24.557	28.406	27.387	1.00 55.05
	60	ATOM	1046	CB	ÀГА	144	23.208	28.947	27.821	1.00 54.70
		MOTA	1047	С	ALA	144	25.637	29.433	27.663	1.00 57.35
		MOTA	1048	0	ALA	144	25.737	29.956	28.780	1.00 58.14

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• •	MOTA	1876	ю.	TRP	1114	51.692	-3.114		1.00 36.42
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76.764
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             2218
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                    CD2 PHE
                              2030
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                    CE1
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                                                 -9.959
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            2224
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                              2030
                                                           75,370
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                    C
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             2226
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	MOTA	2229	CG	PHE	2031	30.474 -13.514	72.317	1.00 28.88
_	ATOM	2230	CD1	PHE	2031	30.614 -12.801	71.139	1.00 28.57
5	ATOM	2231	CD2	PHE	2031	31.616 -13.947	72.981	1.00 28.17
	MOTA	2232	CE1	PHE	2031	31.878 -12.525	70.624	1.00 28.68
	MOTA	2233	CE2	PHE	2031	32.884 -13.676	72.475	1.00 27.81
	MOTA	2234	CZ	PHE	2031	33.017 -12.966	71.297	1.00 27.69
4.0	ATOM	2235	C.	PHE	2031	26.970 -12.926	73.677	1.00 32.61
10	ATOM	2236	0	PHE	2031	26.625 -13.639	74.610	1.00 33.68
	MOTA	2237	N	LEU	2032	26.111 -12.413	72.807	1.00 32.82
	ATOM	2238	CA	LEU	2032	24.694 -12.712	72.924	1.00 32.89
	MOTA	2239	CB	LEU	2032	23.881 -11.873	71.937	1.00 30.95
16	ATOM	2240	CG	LEU	2032	22.373 -12.077	72.055	1.00 30.07
15	ATOM	2241	CD1		2032	21.924 -11.664	73.444	1.00 29.16
	MOTA	2242		LEU	2032	21.652 -11.278	70.990	1.00 28.97
	ATOM	2243	С	LEU	2032	24.514 -14.203	72.633	1.00 33.63
	ATOM	2244	0	LEU	2032	24:999 -14.718	71.618	1.00 33.71
20	ATOM	2245	N	ARG	2033	23.835 -14.903	73.536	1.00 34.59
20	ATOM	2246	CA	ARG.	2033	23.618 -16.329	73.362	1.00 35.19
	ATOM	2247	CB	ARG	2033	24.372 -17.111	74.421	1.00 3472
	ATOM	2248	CG	ARG	2033	24.274 -18.618	74.244	1.00 33.31
	ATOM	.2249	CD	ARG	2033	25.141 -19.334	75.257	1.00 31.04
25.	ATOM	2250	NE	ARG	2033	24.681 -19.100	76.616	1.00 29.30
25 ·	ATOM	2251	CZ	ARG	2033	25.231 -19.668	77.681	1.00 29.82
	ATOM	2252	NH1		2033	26.257 -20.493	77.521	1.00 29.55
	MOTA	2253	NH2		2033	24.761 -19.417	78.897	1.00 29.44
	ATOM	2254	С	ARG	2033	22.164 -16.762	73.375	1.00 36.20
30	ATOM	2255	0	ARG	2033	21.380 -16.371	74,246	1.00 36.24
30	ATOM	2256	N	ILE	2034	21.815 -17.572	72.385	1.00 37.13
	ATOM	2257	CA	TLE	2034	20.473 -18.098	.72.266	1.00 38.70
	ATOM ATOM	2258	CB	ILE	2034	19.895 ~17.795	70.884	1.00 38.45
	ATOM	2259 2260	CG2 CG1		2034	18.493 -18.372	70.777	1.00 37.91
35	ATOM	2261		ILE	2034 2034	19.891 -16.281	70.667	1.00 37.72
<i>J</i> J .	ATOM	2262	CDI	ILE	2034	19.396 -15.847	69.313	1.00 37.52
	ATOM	2263	Ö	ILE	2034	20.544 -19.602 21.110 -20.351	72.510	1.00 39.99
	ATOM	2264		HIS	2035	19.993 -20.037	71.706 73.640	1.00 39-24
	ATOM	2265		HIS	2035	20.043 -21.450	73.840	1.00 41.62
40	ATOM	2266		HIS	2035	20.042 -21.692	75.458	1.00 43.67
	MOTA	2267		HIS	2035	20.808 -22.915	75.857	1.00 44.52 1.00 45.32
	ATOM	2268	CD2		2035		76.131	1.00 45.32
	ATOM	2269	ND1		2035	20.227 -24.166	75.944	1.00 45.72
	MOTA	2270	CE1		2035	21.154 -25.054	76.253	1.00 45.72
45	ATOM	2271	NE2		2035	22.314 -24.432	76.372	1.00 44.96
	ATOM	2272	С	HIS	2035	18.939 -22.240	73.282	1.00 44.91
	ATOM	2273	0	HIS	2035	17.849 -21.720	73.002	1.00 44.68
	ATOM '	2274	Ν.	PRO	2036	19.236 -23.508	72.956	1.00 46.21
	MOTA	2275	CD	PRO	2036	20.598 -24.078	72.880	1.00 46.46
50	ATOM	2276	CA	PRO	2036	18.278 -24.396	72.305	1.00 47.15
•	ATOM	2277		PRO	2036	18.994 -25.730	72.349	1.00 46.84
	ATOM	2278	CG.	PRO	2036	20.398 -25.309	72.016	1.00 46.49
	ATOM	2279	C	PRO	2036	16.902 -24.422	72,959	1.00 48.40
	MOTA	2280	0	PRO	2036	15.885 -24.565	72.272	1.00 48.57
55	MOTA	2281	N .	ASP	2037	16.862 -24.256	74.278	1.00 49.58
	ATOM	2282		ASP	2037	15.591 -24.277	74.995	1.00 51.03
	MOTA	2283		ASP	2037	15.820 -24.763	76.426	1.00 52.08
	ATOM	2284		ASP	2037	16.492 -23.729	77.288	1.00 52.53
<i>c</i> 0	ATOM	2285	OD1		2037	15.777 -22.859	77.826	1.00 52.62
60	ATOM	2286	OD2		2037	17.734 -23.785	77.419	1.00 53.74
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	ATOM	2288	0	ASP	2037	13.784 ~22.826	75.653	1.00 51.96
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	ATOM	3389		ARG	3044		47.578	26.157	76.369	1.00 42.93
	ATOM	3390		ARG	3044		48.401.	24:989	76.870	1.00 43.13
	ATOM	3391		ARG	3044		47.491	24.144	77.729	1.00 42.95
50	ATOM	3392	NE A	ARG	3044		48.096	22.920	78.225	1.00 43.60
	ATOM	3393		ARG	3044	•	48.867	22.850	79.299	1.00 43.94
	ATOM	3394	NH1 2		3044		49.136	23.952	79.989	1.00 44.31
	ATOM	3395	NH2 2	ARG	3044		49.339	21.671	79.700	1.00 43.40
	ATOM	3396	C 2	ARG	3044		46.785	27.573	74.498	1.00 44.18
55	MOTA	3397		ARG	3044		45.740	27.156	74.021	1.00 44.98
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	MOTA	3401	CG (GLU	3045		45.293	32.310	74.475	1.00 51.18
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5	ATOM	3780	CB	PHE	3094	58.234	18.492	57.435	1.00 27.90
,	ATOM ATOM	3781 3782	CG CD1	PHE PHE	3094 3094	59.118 60.093	19.444 18.972	58.176 59.051	1.00 27.67 1.00 27.64
	ATOM	3783		PHE	3094	59.009	20.813	57.975	1.00 27.64
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	ATOM	3785	CE2	PHE	3094	59.852	21.697	58.630	1.00 26.63
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	ATOM	3787	Č	PHE	3094	57.825	17.109	55.440	1.00 29.46
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	ATOM	3798	.C	PHE	3095	55.795	14.931 1 14.669		1.00 29.70
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•	ATOM	3805	OE1	GLU	3096	50.100	17.935	54.990	1.00 23.17
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40	ATOM	3816		ARG	3097	52.360	7.254	55.300	1.00 45.30
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	ATOM	3837	N .	SER	3100	47.841	6.478	61.194	1.00 26.88
•	ATOM	3838	CA	SER	3100	46.683	. 5.630	61.398	1.00 26.68

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	ATOM ATOM	3841 3842	C	SER	3100 3100		45.939	5.957	62.696		26.58
5	MOTA	3843	O N	ASN	3101		44.794 46.581	5.542 6.703	62.887		26.50
•	ATOM	3844	CA	ASN	3101		45.939	7.091	63.590 64.842	1.00	26.11 25.39
	ATOM	3845	CB	ASN	3101		46.969	7.192	65.979	1.00	
	ATOM	3846	CG	ASN	3101		48.100	8.172	65.675		26.77
	ATOM	3847	OD1		3101		47.944	9.099	64.872	1.00	
10	ATOM	3848	ND2		3101		49.247	7.979	66.332		25.52
	ATOM	3849	С	ASN	3101		45.207	8.428	64.685	1.00	25.05
	ATOM	3850	0	ASN	3101		44.718	8.992	65.659		24.75
	ATOM	3851	N	ASN	3102		45.147	8.920	63.451		24.62
15	ATOM ATOM	3852 3853	CA CB	asn Asn	3102 3102		44.482	10.179	63.110		24.62
13	ATOM	3854	CG	ASN	3102		42.192	10.185 9.189	63.626 62.898		24.47 25.74
	ATOM	3855		.ASN	3102		42.040	9.260	61.670		24.41
	ATOM	3856		ASN	3102		41.630	8.236	63.645		26.00
	ATOM	3857	C	ASN	3102		45.169	11.468	63.509		24.41
20	ATOM	3858	0	ASN	3102		44.554	12.525	63.530		.24.40
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	MOTA	3861	CB	TYR	3103		47.992	12.379	65.472		25.19.
25	MOTA	3862	CG	TYR	3103		47.189	12.629	66.724		25.93
25	MOTA '	3863 3864	CD1 CE1		3103 3103		47.022 46.277	13.917 14.141	67.223		26.07
	ATOM	3865	CD2	TYR	3103		46.594	11.567	68.398 67.422		25.99 25.12
	ATOM	3866	CE2		3103		45.861	11.780	68.577		24.25
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30	MOTA	3868	ОН	TYR	3103		44.980	13.263	70.225		25.77
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	MOTA	3870	0	TYR	3103		48.493	11.744	62.312		25.44.
	ATOM	3871	N	ASN	3104		48.724	13.916	62.811		24.40
35	MOTA	3872	CA	ASN	3104		49.694	14.166	61.759		24.50
55	MOTA MOTA	3873 3874	CB CG	ASN ASN	3104 3104		49.471 48.224	15.546 15.620	61.133		23.98
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45	ATOM	3882	OG1	THR	3105		53.921	11.791	60.794	1.00	25.63
73	ATOM ATOM	3883 3884	CG2	THR THR	3105 3105		53.505 54.180	11.585 14.663	63.185 60.976		24.87 26.53
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33	MOTA	3893		TYR	3106		52.131	18.135	61.193		23.99
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                        LEU
                              3118
                                                   19.761
                                                            71.563
                                                                     1.00 34.88
                                                            71.506
70.356
                                                   20.592
21.592
                                                                     1.00
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                                                                           34.02
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                                                                     1.00 33.90
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                        LEU
     MOTA
                    CG
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     MOTA
             4002
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                                          54.215
                                                   22,414
                                                            70.634
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     ATOM
             4003
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                              3118
                                          56.670
                                                  .22.518
                                                            70.225
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                                          56.953
     ATOM
             4004
                    C
                        LEU
                              3118
                                                   18.943
                                                            72.846
                                                                     1.00 36.89
                                                                     1.00 37.67
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                                                            72.897
     ATOM
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                        LEU
                              3118
                                          56.347
                                          57.650
                                                            73.871
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             4006
                    N
                        LYS
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                                                   19.431
                                                                     1.00 38.85
45
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                                          57.707
                                                   18.747
                                                            75.158
                                                                     1.00 40.71
     MOTA
                    CA
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                                                   19.149
                                                            75.934
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                    CB
                        LYS
                              3119
                                                                     1.00 42.18
     MOTA
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                        LYS
                              3119
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                                                   18.648
                                                            75.320
                                                                     1.00 44.83
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76.790
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                        LYS
                              3119
                                                                     1.00 46.30
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                                          61.898
                                                   19.910
                                                                     1.00 48.37
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                                                   19.141
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                                                                     1.00 41.75
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56.237
                                                            75.590
77.069
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                              3119
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                                                   18.443
                                                                     1.00 43.43
                    N
                        ARG
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                        ARG
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                                                   18.737
                                                            77.939
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                                                   17.720
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                                                            79.084
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                        ARG
     ATOM
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                    NE
                        ARG
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                                                   13.990
                                                            79.629
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                                                                           56.91
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                                                            80.467
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                    NH1 ARG
                              3120
                                          55.175
                                                   13.145
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                                                                           57.86
     ATOM
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                    NH2 ARG
                              3120
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                                                   11.757
                                                            80.145
                                                                     1.00
                                                                          58.75
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     ATOM
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	ATOM	4025	0	ARG	3120		54.240	20.665	79.099	1.00 45.78	
	ATOM	4026	N	THR	3121		6.402	20.738	78.463	1.00 45.18	
	ATOM	4027	CA	THR	3121	-	6.628	22.067	79.027	1.00 43.90	
	ATOM	4028	СВ	THR	3121		8.092	22.278	79.410	1.00 43.45	
5	ATOM	4029	OG1		3121		8.898	22.262	78.228	1.00 43.56	
	ATOM	4030	CG2		3121		8.560	21.190	80.342	1.00 43.10	
•	ATOM	4031	C	THR	3121		6.257	23.172	78.061	1.00 43.77	
	ATOM	4032	ŏ	THR	3121		6.225	24.335	78.429	1.00 43.80	
	ATOM	4033	Ŋ	GLY	3122		55.975	22.811	76.819	1.00 44.12	
10	ATOM	4034	CA	GLY	3122		5.633	23.820	75.837	1.00 43.82	
- 0	ATOM	4035	Č.	GLY	3122		6.854	24.228	75.036	1.00 43.46	
	ATOM	4036	ŏ	GLY	3122		6.759	25.036	74.119	1.00 43.46	
	ATOM	4037	N	GLN	3123	•	8.006	23.683	75.399	1.00 43.38	
	ATOM	4038	CA	GLN	3123		9.242	23.965	74.687	1.00 43.16	
15	ATOM	4039	CB	GLN	3123	_	0.438	23.903	75.630		
13	ATOM	4040	CG.	GLN	3123		0.456	24.946		1.00 43.92	
	ATOM	4041	CD	GLN	3123				76.669	1.00 44.98	
	ATOM	404.1	OE1		3123		0.512	26.322	76.045	1.00 46.14	
							1.441	26.653	75.303	1.00 46.76	
20	MOTA	4043	NE2		3123		9.505	27.135	76.336	1.00 46.90	
20	MOTA	4044	C	GLN	3123		9.372	22.907	73.606	1.00 43.11	
	MOTA	4045	0	GLN	3123		8.953	21.770	73.802	1.00 43.38	
	MOTA	4046	N	TYR	3124			.23.267	72.468	1.00 42.36	
	ATOM	4047	CA	TYR	3124		0:102	22.298	71.399		
25	ATOM	4048	CB	TYR	3124		0.657	22.981	70.142	1.00 41.81	
25	ATOM	4049	CG	TYR	3124		2.136	23.312	70.187	1.00 41.67	
•	ATOM	4050		TYR	3124		3.097		70.021	1.00 41.76	
	ATOM	4051	CE1		3124		4.456	22.606	70.054	1.00 42.16	
	ATOM	4052	CD2		3124		2.574	24.623	70.390	1.00 41.60	
00	ATOM	4053	CE2		3124		3.932	24.931	70.427	1.00 41.64	
30	ATOM ·		CZ	TYR	3124		4.870	23.917	70.258	1.00 42.45	
•	ATOM	4055	ОН	TYR	3124		6.221	24.203	70.295	1.00 42.72	
	MOTA	4056	С	TYR	3124		1.043	21.205	71.875	1.00 41.62	
	ATOM	4057	0	TYR	3124		1.831	21.424	72.788	1.00 42.04	
~ -	MOTA	4058	N	LYS	3125		0.953	20.031	71.265	1.00 41.16	
35.	ATOM	4059	CA	LYS	3125		1.810	18.914	71.631	1.00 40.81	
	MOTA	4060	CB	LYS	3125	6	0.956	17.674	71.900	1.00 39.63	
	ATOM	4061	·CG	LYS	3125	6	1.740	16.428	72.229	1.00 38.43	
	ATOM	4062	CD	LYS	3125	6	0.819	15.299	72.630	1.00 37.98	
	MOTA	4063	CE	LYS	3125	6	1.606	14.045	72.984	1.00 38.56	
40	ATOM	4064	NZ	LYS	3125	6	0.771	12.994	73.632	1.00 36.78	
	ATOM	4065	C	LYS	3125	6	2.793	18.646	70.496	1.00 41.13	
	ATOM	4066	0	LYS	3125	6	2.401	18.593	69.334	1.00 41.25	
	ATOM	4067	N	LEU	3126	. 6	4.070	18.500	70.833	1.00 41.40	
	ATOM	4068	CA	LEU	3126	6	5.098	.18.233	69.838	1.00 41.51	
45	ATOM	4069	CB	LEU	3126	6	6.416	17.905	70.533	1.00 41.76	
•	ATOM	4070	CG	LEU	3126	6	7.049	19.067	71.296	1.00 42.64	
	ATOM	4071	CD1	LEU	3126		8.235	18.565	72.099	1.00 42.24	
	ATOM	4072	CD2	LEU	3126		7.473	20.147	70.313	1.00 42.13	
	ATOM	4073	С	LEU	3126	6	4.709	17.076	68.924	1.00 41.69	
50	ATOM	4074	0	LEU	3126	6	4.354	15.996	69.397	1.00 42.10	
	ATOM	4075	N	GLY	3127		4.781	17.301	67.616	1.00 41.22	
	ATOM	4076	CA	GLY	3127		4.439	16.253	66.679	1.00 41.14	
	ATOM	4077	C	GLY	3127		5.301	15.028	66.899	1.00 41.67	
	ATOM	4078	ŏ	GLY	3127		4.864	13.895	66.686	1.00 41.09	
55	ATOM	4079	N	SER	3128		6.535	15.259	67.336	1.00 42.01	
	ATOM	4080	CA	SER .			7.473	14.172	67.578	1.00 42.37	
	ATOM	4081	CB	SER	3128		8.845	14.746	67.930	1.00 42.37	
	ATOM	4082	OG	SER	3128		8.801	15.447	69.160		
	ATOM	4083	C	SER	3128		6.993	13.267	68.709	1.00 41.94	
60	ATOM	4084	o	SER	3128		7.455			1.00 42.59	
50	ATOM	4085	N	LYS.			6.056	12.140 13.769	68.851 69.504	1.00 41.75	
	ATOM	4085	CA	LYS .						1.00 43.34	
	ATOM	4000	CA.	nro	3129	ь	5.532	13.022	70.642	1.00 44.33	

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	MOTA	4087	CB	LYS	3129		65.479	13.952	71.876	1.00 45.33
	MOTA	4088	CG	LYS	3129		65.888	13.310	73.208	1.00 48.32
	MOTA	4089	CD	LYS	3129		64.848	13.517	74.349	1.00 50.22
_	ATOM	4090	CE	LYS	3129		64.795	14.969	74.876	1.00 51.56
5	ATOM	4091	NZ	LYS	3129		63.774	15.190	75.960	1.00 51.30
	ATOM	4092	C	LYS ·	3129		64.135	12.458	70.359	1.00 43.96
	ATOM	4093	0	LYS	3129		63.532	11.830	71.231	1.00 44.17
	ATOM	4094	N	THR	3130		63,622	12.676	69.149	1.00 43.04
10	ATOM	4095	CA	THR	3130		62.284	12.201	68.803	1.00 42.15
10	ATOM	4096 4097	CB	THR THR	3130 3130		61.622	13.122	67.759	1.00 41.22
	ATOM ATOM	4097		THR	3130		62.384 61.549	13.093 14.551	66.548 68.275	1.00.40.88
	MOTA	4099	C	THR	3130		62.282	10.771	68.275	1.00 40.27
	ATOM	4100	õ	THR	3130		63.329	10.771	67.959	1.00 42.10
15	ATOM	4101	N	GLY	3131		61.095	10.184	68.193	1.00 41.80
	ATOM	4102	CA	GLY	3131		60.963	8.827	67.701	1.00 41.29
	ATOM	4103	C	GLY	3131		59.516	8.552	67.345	1.00 41.14
	MOTA	4104	0	GLY	3131		58.632	9.306	67.757	1.00 40.85
	ATOM	4105	N	PRO	3132		59.235	7.484	66.581	1.00 41.29
20	ATOM	4106	CD	PRO	3132		60.210	6.577	65.957	.1.00 41.74
	ATOM	4107	CA	PRO	3132		57.873	7.126	66.175	1.00 41.21
	ATOM	4108	CB	PRO	3132		58.088	5.937	65.233	1.00 41.09
	ATOM	4109	CG	PRO	3132		59.367	5.354	65.693	-1·.00 41.75
05	ATOM	4110	Ç	PRO	3132		56.884	6.829	67.302	1.00 41.23
25	ATOM	4111	0	PRO	3132		55.699	7.157	67.192	1.00 41.41
	MOTA	4112	N	GLY	3133		57.361	6.227	68.386	1.00 40.72
	ATOM	4113 4114	CA	GLY	3133		56.469	5.917	69.488	1.00 40.27
	MOTA MOTA	4114	C	GLY.	3133 3133		56.308	7.018 6.734	70.521	1.00 39.61 1.00 40.41
30 ·	ATOM	4115	O N	GLY	3134		56.019 56.476	8.271	71.684 70.113	1.00 38.20
50	ATOM	4117	CA	GLN	3134	٠.	56.357	9.374	71.053	1.00 37.29
	ATOM	4118	CB	GLN	3134		57.595	10.259		1.00 37.29
	ATOM	4119	CG	GLN	3134		58.879	9.556		1.00 35.59
_	ATOM	4120	CD	GLN	3134		60.042	10.513	71.353	1.00 36.21
35	MOTA	4121	OE1	GLN .	3134		61.191	10.117	71.528	1.00 36.13
	MOTA	4122	NE2	GLN	3134		59.749	11.790	71.161	1.00 35.89
	ATOM	4123	С	GLN	3134		55.117	10.227	70.849	1.00 37.01
	ATOM	4124	0	GLN	3134		54.692	10.480	69.733	1.00 37.74
40	ATOM	4125	N	LYS	3135		54.551	10.674	71.956	1.00 36.45
40	ATOM	4126	CA	LYS	3135		53.363	11.507	71.969	1.00 35.39
	ATOM	4127	CB	LYS	3135		52.826	11.513	73.396	1.00 35.38
	ATOM	4128	CG	LYS	3135		51.563	12.276	73.664	1.00 35.73
	ATOM	4129	CD	LYS	3135		51.176	11.987	75.102	1.00 36.00
45	ATOM ATOM	4130 4131	CE NZ	LYS LYS	3135 3135		49.882 49.652	12.643	75.510 76.968	1.00 37.40
43	ATOM	4132	C	LYS	3135		53.701	12.408 12.925	70.900	1.00 38.21 1.00 35.02
	MOTA	4133	õ	LYS	3135		52.839	13.650	71.028	1.00 35.67
	ATOM	4134	N	ALA	3136		54.967	13.302	71.683	1.00 33.63
	ATOM	4135	CA	ALA	3136		55.451	14.628	71.332	1.00 32.46
50	ATOM	4136	СВ	ALA	3136		56.836	14.820	71.909	1.00 32.39
-	ATOM	4137	C	ALA	3136		55.468	14.961	69.839	1.00 32.06
	MOTA	4138	0	ALA	3136		55.460	16.139	69.460	1.00 32.00
	ATOM	4139	N	ILE	3137		55.486	13.942	68.986	1.00 30.71
	ATOM	4140	CA	ILE	3137		55.522	14.197	67.549	1.00 29.93
55	ATOM	4141	CB	ILE	3137		56.356	13.132	66.809	1.00 28.69
	ATOM	4142	CG2		3137		57.734	12.991	67.469	1.00 26.72
	ATOM	4143	CG1		3137		55.587	11.813	66.775	1.00 27.75
	ATOM	4144	CD1		3137		56.247	10.726	65.958	1.00 26.34
60	ATOM	4145	C	ILE	3137	_	54.149	14.260	66.880	1.00 30.23
60 .	ATOM	4146	0.	ILE	3137	•	54.053	14.573	65.695	1.00 30.59
	ATOM	4147	N	LEU	3138		53.095	13.982	67.641	1.00 29.89
•	ATOM	4148	CA	LEU	3138		51.742	13.971	67.099	1.00 29.30

	ATOM ATOM	4149 4150	CB CG	LEU LEU	3138 3138		50.913 51.579	12.926 11.552	67.835 67.799		28.78 28.96
	MOTA	4151	CD1	LEU	3138		50.814	10.552	68.659		28.80
_	MOTA	4152	CD2	LEU	3138		51.638	11.093	66.343	1.00	30.05
5	MOTA	4153	С	LΕU	3138		51.014	15.308	67.146		29.53
	ATOM	4154	0	LEU	3138		50.895	15.931	68.204		29.55
	ATOM	4155	N	PHE	3139		50.506	15.746	65.998		28.97
	ATOM	4156	CA	PHE	3139 3139		49.777	17.006	65.948		28.49
10	ATOM ATOM	4157 4158	CB CG	PHE PHE	3139		50.557 51.850	18.075 18.436	65.188 65.822		27.65 25.80
10	ATOM	4159		PHE	3139		52.962	17.632	65.654		25.85
	ATOM	4160		PHE	3139		51.949	19.567	66.615		26.05
	ATOM	4161		PHE	3139		54.152	17.948	66.265		26.07
	ATOM	4162	CE2	PHE	3139		53.136	19.892	67.229		25.33
15	MOTA	4163	CZ	PHE	3139		54.239	19.083	67.056	1.00	26.10
	ATOM	4164	C	PHE	3139		48.428	16.864	65.301		29.32
	ATOM	4165	0	PHE	3139		48.255	16.120	64.342		29.93
	ATOM	4166	N	LEU	3140		47.473	17.610	65.826		29.75
20	ATOM ATOM	4167 4168	CA CB	LEU	3140 3140		46.125 45.146	17.583 17.408	65.310 66.473		30.88
20	ATOM	4169	CG	LEU	3140		43.700	17.032			30,22 29.88
	ATOM	4170		LEU	3140		43.700	15.831			29.65
	ATOM	4171		LEU	3140		42.941	16.735	·67.434		29.30
•	ATOM	4172	С	LEU	3140		45.900	18.910			32.12 .
25	MOTA	4173	0	LEU	3140		45.879	19.953	65.250	1.00	32.46
	ATOM .	4174	N	PRO	3141		45.753	18.891	63.277		32.93
	ATOM	4175	CD.	PRO	3141 .		45.750	17.734	62.366		33.53
	ATOM	4176	CA.	PRO	3141		45.535	20.134	62.542		34.24
30	ATOM ATOM	4177 4178	CB	PRO PRO	3141 3141		45.755 45.177	19.710 18.324	61.095 61.093		33.67
JU .	ATOM	4179	CG C	PRO	31.41	•	44.135	20.682	62.791		33.64 35.81
	ATOM	4180	Ö	PRO	3141		43.158	19.944	62.758		35.58
	ATOM	4181	N	MET	3142		44.046	21.978	63.056		37.82
	ATOM	4182	CA	MET	3142		42.762	22.625	63.296		40.51
35	ATOM	4183	CB	MET	31.42		42.628	23.014	64.757	1.00	39.85
•	ATOM	4184	.CG	MET	3142			.21.894	65.702		41.10
	ATOM	4185	SD	MET	3142		42.525	22.404	67.380		42.03
	MOTA	4186	CE	MET	3142		40.829	22.046	67.466		42.50
40	ATOM ATOM	4187. 4188	0	MET MET	3142· 3142		42.698 43.715	23.887	62.464 62.260		42.36 42.88
40	ATOM	4189	N	SER	3143		41.515	24.240	61.985		44.85
•	ATOM	4190	CA	SER	3143		41.394	25.452	61.194		47.93
	.ATOM	4191	CB	SER	3143		39.985	25.599	60.633		48.53
	ATOM	4192	OG	SER	3143		39.051	25.849	61.670		50.73
45	ATOM	4193	С	SER	3143		41.715	26.632	62.101		49.87
	MOTA	4194	0	SER	3143		41.570	26.548	63.328		49.27
	MOTA	4195	N	ALA	3144			27.720	61.496		52.56
	ATOM	4196	CA	ALA	3144		42.517	28.920	62.248		55.28
50	ATOM ATOM	4197 4198	CB	ALA ALA	3144 3144		43.839	29.490 29.896	61.769		54.86
50	ATOM	4199	0	ALA	3144		41.372	30.592	61.987 60.976	1 00	58.54
	ATOM	4200	N	LYS	3145		40.404	29.880	62.869		60.39
•	ATOM	4201	CA	LYS	3145		39.257	30.751	62.729		62.90
	ATOM	4202	CB	LYS	3145		38,129	30.018	61.977		64.47
55	MOTA	4203	CG	LYS	3145		38.583	29.441	60.617	1.00	66.36
	ATOM	4204	CD	LYS	3145		37.443	28.879	59.756		67.43
	ATOM	4205	CE	LYS	3145		37.979	28.357	58.411		67.94
	MOTA	4206	NZ	LYS	3145		36.907	27.887	57.477		68.21
60	ATOM	4207	C	LYS	3145		38.854	31.126	64.144		63.85
UU	ATOM ATOM	4208 4209	O N	LYS ALA	3145 3146		38.323 39.153	30.297 32.379	64.895 64.487		63.55 64.80
	ATOM	4210	CA	ALA	3146		38.897	32.373	65.796		66.21
					J= - V		50.55		33.730	2.00	

	ATOM	4211	СВ	ALA	3146		20 147	22 010	66 736	1 00 66 07
	ATOM	4211		ALA	3146		38.147	32.019	66.736	1.00 66.07
			C	ALA	3146		40.254	33.341	66.397	1.00 66.79
	ATOM	4213	0				41.256	33.074	65.694	1.00 67.66
5	ATOM	4214	CB	MSE	2149		27.593		-21.743	1.00 75.07
3	ATOM	4215	CG	MSE	2149		26.822		-21.312	1.00 78.40
	ATOM	4216	SE	MSE	2149		26.886		~22.467	1.00 83.46
	ATOM	4217	CE	MSE	2149		25.367		-23.446	1.00 81.31
	MOTA	4218	C	MSE	2149		29.613		-20.303	1.00 71.30
	ATOM	4219	0	MSE	2149		28.993	19.709	-19.300	1.00 71.53
10	ATOM	4220	N	MSE	2149		29.736	18.408	-22.143	1.00 72.18
	ATOM	4221	CA	MSE	2149		29.125	19.699	-21.714	1.00 72.61
	ATOM	4222	N	PRO	2150		30.731	20.811	-20.217	1.00 69.63
	ATOM	4223	CD	PRO	2150		31.405	21.382	-21.394	1.00 69.49
	ATOM	4224	CA	PRO	2150		31.375	21.273	-18,977	1.00 68.16
15	ATOM	4225	CB	PRO	2150		32.479	22,200	-19.479	1.00 68.32
	ATOM	4226	CG	PRO	2150		32.777		-20.850	1.00 69.55
	ATOM	4227	c	PRO	2150		30.460		-18.014	1.00 66.65
	ATOM	4228	Ö	PRO	2150		29.831		-18.395	1.00 66.56
	ATOM	4229	N	VAL	2151		30.405		-16.766	1.00 64.70
20	ATOM	4230	CA	VAL	2151				-15.751	1.00 62.62
20	ATOM	4231	CB	VAL	2151.		28.297			
	ATOM	4232					27.428		-15.496	1.00 62.77
			CG1	VAL	2151 2151				-14.511	.1.00 62.32
	ATOM	4233	CG2	VAL			27.568		-16.807	1.00:62.65
25	ATOM	4234	C	VAL	2151		30.342		-14.433	1.00 61.28
23	ATOM	4235	0	VAL	2151		30.806		-13.870	1.00 61.55
	MOTA	4236	N	ALA	2152		30.476		-13.955	1.00 59.27
	ATOM.	4237	CA	ALA	2152		31.163		-12.696	1.00 57.33
•.	ATOM	4238	CB	ALA	2152		31.343		-12.496	1.00 56.70
	ATOM	4239	С	ALA	2152	•	30.321		-11.562	1.00 56.10
30 .	ATOM	4240	0	ALA	2152	•	29.087		-11.594	1.00 55.91
•	ATOM	4241	N	PRO	2153		30.980	22.678	-10.535	1.00 54.52
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	ATOM.	4243	CA	PRO	2153		30.318	22.060	-9.379	1.00 52.93
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35	ATOM	4245	CG	PRO	2153		32.480	22.853	-8.790	1.00 53.56
	MOTA	4246	Ç.	PRO	2153	•	29.186	22.853	-8.739	1.00 51.17
	ATOM	4247	0	PRO	2153		29.262	24.065	-8.591	1.00 51.17
	ATOM	4248	N	TYR	2154		28.132	22.143	-8.365	1.00 49.67
	ATOM	4249	CA	TYR	2154		26.966	22.751	-7.733	1.00 48.69
40	MOTA	4250	CB	TYR	2154		25.940	23.170	-8.799	1.00 47.37
	ATOM	4251	CG	TYR	2154		25.395	22.015	-9.622	1.00 46.49
	ATOM	4252	CD1	TYR	2154		26.202	21.343	-10.548	1.00 45.55
	ATOM	4253	CE1	TYR	2154		25.721		-11.272	1.00 45.14
	ATOM	4254	CD2	TYR	2154		24.087	21.564	-9.445	1.00 46.44
45	ATOM	4255	CE2	TYR	2154		23.595		-10.165	1.00 46.07
	ATOM	4256	CZ	TYR	2154		24.419		-11.072	1.00 45.55
	ATOM	4257	ОН	TYR	2154		23.949		-11.748	1.00 44.58
	ATOM	4258	C.	TYR	2154		26.321	21.749	-6.765	1.00 48.29
	ATOM		ŏ	TYR	2154)	26.421	20.537	-6.950	1.00 47.58
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	MOTA	4261	CA	TRP	2155		24.997	21.413	-4.761	1.00 47.39
	MOTA	4262	CB	TRP	2155		24.578	22.235	-3.541	1.00 45.56
	ATOM	4263	CG	TRP	2155		25.696	22.971	-2.860	1.00 43.22
55	ATOM	4264	CD2		2155		26.939	22.425	-2.403	1.00 41.64
55	ATOM	4265	CE2		2155		27.659	23.476	-1.801	1.00 41.47
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	ATOM	4269	CZ2		2155		28.926	23.294	-1.242	1.00 41.05
60	ATOM	4270	CZ3		2155	•	28.778	20.970	-1.889	1.00 40.72
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5	ATOM	4339	CA	LYS	2164	25.163	23.619	10.185	1.00 46.14
•	ATOM	4340	CB	LYS	2164	25.463	25.095	9.915	1.00 47.42
	ATOM	4341	CG	LYS	2164	25.304	25.459	8.428	1.00 49.19
	ATOM	4342	ÇD	LYS	2164	26.100	26.704	8.055	1.00 51.03
	ATOM	4343	CE	LYS	2164	27.584	26.543	8.405	1.00 51.49
10	ATOM	4344	NZ	LYS	2164	28.423	27.692	7.949	1.00 51.95
	ATOM	4345	C	LYS	2164	25.820	23.135	11.476	1.00 44.65
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15	ATOM	4349	CB	LEU	2165	25.338	23.700	15.042	1.00 38.84
	ATOM	4350	CG	LEU	2165	25.670	23.090	16.416	1.00 37.93
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	ATOM	4353	Ç	LEU		25.219	21.385	14.177	1.00 38.63
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	ATOM	4357	ĊB	HIS	.2166	26.517	18.067	13:813	1.00 36.60
	ATOM	4358	CG	HIS	2166	25.967	17.966	12.419	1.00 38.11
25	ATOM	4359		HIS	2166	25.856	18.885	11.426	1.00 38.56
	MOTA	4360		HIS	2166.	25.518	16.774	11.883	1.00 38.28
	MOTA	4361		HIS	2166	25.154	16.964	10.625	1.00 37.67
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	ATOM	4363	C	HIS	2166	26.310	18.904	16.139	1.00 35.15
30	ATOM	4364	Ó	HIS	2166	27.520	18:896	16.392	1.00 35.14
-	ATOM	4365	N	ALA	2167	25.378	18.769	17,071	1.00 33.33
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	ATOM	4368	С	ALA	2167	25.308	17.144	18.809	1.00 30.13
35	ATOM	4369 .	0	ALA	2167	24.183	16.744	18.531	1.00 30.31
	ATOM	4370	N	VAL	2168	26.206	16.375	19.398	1.00 29.06
	ATOM	4371	CA	VAL	2168	25.875	15.009	19.768	1.00 27.84
	MOTA	4372	CB	VAL	2168	26.288	14.010	18.674	1.00 28.12
	MOTA	4373	CG1	VAL	2168 .	25.514	14.265	17.401	1.00 28.23
40	MOTA	4374	CG2	VAL	2168	27.782	14.119	18.429	1.00 27.63
	MOTA	4375	С	VAL	2168	26.601	14.580	21.021	1.00 26.89
٠.	MOTA	4376	0	VAL	2168	27.626	15.155	21.389	1.00 27.64
	MOTA	4377	N	PRO	2169 .	26.071	13.563	21.697	1.00 26.04
4-	MOTA	4378	CD	PRO	2169	24.781	12.890	21.451	1.00 26.22
45	MOTA	4379	CA	PRO	2169	26.712	13.067	22.911	1.00 26.17
	MOTA	4380	CB	PRO	2169	25.624	12.191	23.527	1.00 25.80
	MOTA	4381	CG	PRO	2169	24.875	11.675	22.324	1.00 25.68
	MOTA	4382	С	PRO	2169	27.924	12.272	22.435	1.00 26.20
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50	MOTA	4384	N	ALA	2170	28.904	12.074	23.305	1.00 26.35
•	MOTA	4385	CA	ALA	2170	30.088	11.310	22.953	1.00 26.76
	MOTA	4386	CB	ALA	2170	31.017	11.271	24.140	1.00 25.11
	MOTA	4387	C	ALA	2170	29.714	9.888	22.532	1.00 26.88
~~	MOTA	4388	0	ALA	2170	28.696	9.354	22.965	1.00 27.39
55	ATOM	4389	N	ALA	2171	30.530	9.294	21.667	1.00 27.36
	ATOM	4390	CA	ALA	2171	30.336	7.912	21.207	1.00 27.41
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•	ATOM	5158	С	ALA	2268		28.175	32.038	69.214	1.00	
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.35	ATOM	5174	CB	SER	2271		28.051	33.476	65.256		47.64
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	ATOM	5178	И О	SER ASN	2271 2272		24.871	33.616	64.151		47.41
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40	ATOM	5180	СВ	ASN	2272		25.808	35.348	61.622 60.705		46.45
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J Q	ATOM	5191	C	VAL VAL	2273 2273		27.228	28.429	60.016		46.19
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ATOM 5576 N GLU 2322 20.717 29.850 44.488 1.00 41.77 ATOM 5577 CA GLU 2322 19.905 30.997 46.437 1.00 42.24 ATOM 5578 CB GLU 2322 19.905 30.997 46.437 1.00 42.26 ATOM 5580 CD GLU 2322 17.515 31.730 46.309 1.00 48.52 ATOM 5581 CB GLU 2322 17.515 31.730 46.309 1.00 48.52 ATOM 5581 CB GLU 2322 17.000 32.296 45.314 1.00 49.41 ATOM 5582 CB GLU 2322 17.000 32.296 45.314 1.00 49.41 ATOM 5583 C GLU 2322 20.785 27.13 46.709 1.00 41.07 ATOM 5584 C GLU 2322 20.785 27.13 46.709 1.00 41.07 ATOM 5586 C GLU 2322 20.785 28.713 46.709 1.00 41.07 ATOM 5586 CA MSE 2323 20.586 25.713 46.003 1.00 39.61 ATOM 5586 CA MSE 2323 20.580 26.319 46.848 1.00 37.68 ATOM 5586 CA MSE 2323 19.309 25.575 40.003 1.00 39.61 ATOM 5587 CB MSE 2323 19.309 25.575 40.003 1.00 35.05 ATOM 5580 CC MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5590 CB MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5591 C MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5592 C MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5595 CB GLU 2324 22.376 26.195 46.882 1.00 38.50 ATOM 5596 CB GLU 2324 22.376 26.195 46.882 1.00 38.50 ATOM 5596 CB GLU 2324 22.376 26.195 46.882 1.00 38.50 ATOM 5596 CB GLU 2324 22.376 26.195 46.882 1.00 38.50 ATOM 5596 CB GLU 2324 22.376 26.195 46.882 1.00 38.57 ATOM 5596 CB GLU 2324 22.376 26.195 46.882 1.00 38.57 ATOM 5596 CB GLU 2324 24.230 25.636 47.352 1.00 38.57 ATOM 5596 CB GLU 2324 24.330 25.636 47.352 1.00 38.57 ATOM 5596 CB GLU 2324 24.330 25.636 47.352 1.00 38.57 ATOM 5598 CB GLU 2324 26.613 25.503 43.770 1.00 40.77 ATOM 5598 CB GLU 2324 26.613 25.503 43.770 1.00 40.79 ATOM 5598 CB GLU 2324 26.613 25.503 43.770 1.00 40.79 ATOM 5598 CB GLU 2324 26.613 25.503 43.770 1.00 40.39 ATOM 5598 CB GLU 2324 26.613 25.503 29.545 51.00 39.93 ATOM 5598 CB GLU 2324 26.597 23.522 30.39 50.355 1.00 39.93 ATOM 5598 CB GLU 2324 26.597 23.522 30.39 50.355 1.00 39.93 ATOM 5598 CB GLU 2324 26.597 23.50 ATOM 5598 CB GLU 2324 26.597 23.50 ATOM 5598 CB GLU 2324 26.597 23.50 ATOM 5598 CB GLU 2324 26.5		ATOM	5575	0	LYS	2321		22.778	30.557	44.002	1.00 41.17
ATOM 5577 CR GLU 2322 20,910 29,986 45,920 1,00 42,24 ATOM 5579 CG GLU 2322 18,503 30,623 46,045 1,00 46,69 ATOM 5580 CD GLU 2322 17,261 32,034 47,503 1,00 48,52 ATOM 5581 DEI GLU 2322 17,261 32,034 47,503 1,00 49,41 ATOM 5582 CD 2GLU 2322 17,261 32,034 47,503 1,00 49,41 ATOM 5583 C GLU 2322 20,785 28,771 47,793 1,00 41,26 ATOM 5584 C GLU 2322 20,785 28,771 47,793 1,00 41,26 ATOM 5585 N MSE 2323 20,867 27,561 46,103 1,00 39,61 ATOM 5586 CM SSE 2323 19,806 25,275 46,603 1,00 39,61 ATOM 5586 CM SSE 2323 19,806 25,275 46,603 1,00 39,61 ATOM 5587 CB MSE 2323 19,806 25,275 46,603 1,00 35,08 ATOM 5589 SE MSE 2323 17,386 25,273 45,788 1,00 30,55 ATOM 5590 CC MSE 2323 17,386 25,726 47,320 1,00 25,96 ATOM 5590 CM SSE 2323 17,386 25,726 47,320 1,00 25,96 ATOM 5590 CM SSE 2323 17,386 25,726 47,320 1,00 25,96 ATOM 5590 CM SSE 2323 17,386 25,726 47,320 1,00 25,96 ATOM 5590 CM SSE 2323 17,386 25,726 47,320 1,00 25,96 ATOM 5590 CM SSE 2323 17,386 25,726 47,320 1,00 38,50 ATOM 5590 CM SSE 2323 17,386 25,726 47,320 1,00 38,50 ATOM 5590 CM SSE 2323 12,807 24,899 44,226 1,00 38,50 ATOM 5590 CM GGLU 2324 22,976 26,195 46,882 1,00 38,50 ATOM 5590 CM GLU 2324 22,976 26,195 46,882 1,00 38,50 ATOM 5590 CM GLU 2324 22,976 26,195 46,882 1,00 38,50 ATOM 5590 CM GLU 2324 22,300 24,489 44,216 1,00 40,09 ATOM 5601 CM GLU 2324 26,230 24,489 44,216 1,00 40,09 ATOM 5600 CM QLU 2324 26,590 27,583 36,700 1,00 39,48 ATOM 5600 CM QLU 2324 26,590 27,583 36,700 1,00 39,48 ATOM 5600 CM QLU 2324 26,590 27,583 36,700 1,00 39,49 ATOM 5600 CM QLU 2324 26,590 27,583 29,545 1,00 39,49 ATOM 5600 CM QLU 2324 26,590 27,585 31,687 1,00 39,49 ATOM 5600 CM QLU 2324 26,590 27,583 29,545 1,00 39,49 ATOM 5600 CM QLU 2324 26,590 27,583 29,545 1,00 39,49 ATOM 5600 CM QLU 2324 26,590 27,583 29,545 1,00 39,49 ATOM 5600 CM QLU 2324 26,590 27,583 29,545 1,00 39,49 ATOM 5600 CM QLU 2324 27,550 22,560 47,590 1,00 39,49 ATOM 5600 CM QLU 2324 27,50 22,50 5,533 29,545 1,00 39,49 ATOM 5600 CM QLU 2324 27,50 22,50 5,50 3,50 1,00 39,49 ATOM 5600 CM QLU 2324 27,50 22,50 5,50 3,50		MOTA	5576	N	GLU	2322		20.717	29.850	44.488	1.00 41.77
S		ATOM		CA	GLU	2322		20.910	29.986	45.920	
5 ATOM 5580 CD GLU 2322		ATOM	5578	CB	GLU	2322		19.905	30.997	46.437	
ATOM 5580 CD GEU 2322 17.515 31.730 46.309 1.00 48.52 ATOM 5581 CG GLU 2322 17.261 32.034 47.503 1.00 49.41 ATOM 5583 CG GLU 2322 20.785 28.713 46.749 1.00 41.07 ATOM 5583 CG GLU 2322 20.785 28.713 46.749 1.00 41.07 ATOM 5583 CG GLU 2322 20.785 28.713 46.749 1.00 41.07 ATOM 5585 CG GLU 2322 20.785 28.713 46.749 1.00 41.07 ATOM 5586 CA MSE 2323 20.687 27.561 46.103 1.00 39.61 ATOM 5586 CA MSE 2323 20.538 26.339 46.848 1.00 37.88 ATOM 5586 CG MSE 2323 19.806 25.275 46.003 1.00 35.05 ATOM 5588 CG MSE 2323 19.806 25.275 46.003 1.00 35.05 ATOM 5580 CE MSE 2323 19.806 25.275 46.003 1.00 35.05 ATOM 5580 CE MSE 2323 17.396 25.725 47.300 10.00 26.31 ATOM 5590 CE MSE 2323 17.396 25.725 47.300 10.00 26.31 ATOM 5590 CE MSE 2323 17.396 25.725 47.300 10.00 26.31 ATOM 5593 CM MSE 2323 21.835 25.722 47.365 1.00 38.50 ATOM 5593 CM GLU 2324 22.876 22.835 46.882 1.00 38.50 ATOM 5595 CG GLU 2324 22.8976 22.636 47.352 1.00 38.50 ATOM 5595 CG GLU 2324 22.8976 26.195 46.882 1.00 38.50 ATOM 5595 CG GLU 2324 25.895 25.663 46.253 1.00 39.58 ATOM 5599 CE GLU 2324 25.027 24.499 44.216 1.00 40.77 ATOM 5590 CC GLU 2324 26.830 24.499 44.216 1.00 39.58 ATOM 5590 CC GLU 2324 25.895 25.668 46.881 1.00 39.43 ATOM 5601 C GLU 2324 25.895 25.668 46.881 1.00 39.43 ATOM 5600 C GLU 2324 25.897 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 25.897 23.322 43.943 1.00 39.49 ATOM 5600 C GLU 2324 25.503 29.039 50.355 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.69 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 25.503 29.395 50.555 1.00 39.99 ATOM 5600 CG U 2324 2325 23.966 55.255 1.00 39.99 ATOM 5600 CG U 2324 2325 23.966 55.255 1.00 39.99 ATOM 5600 CG U 2324 2325 23.966 55.255 1.00 39.99 ATOM 5600 CG U 2326 23.955 1.00 30.355 1.00 39.99 ATOM 5600 CG U 2326 23.95	5	ATOM	5579	CG	GLU	2322		18.503	30.623	46.045	1.00 46.69
ATOM 5581 OE1 GLU 2322 17.261 32.034 47.503 1.00 49.41 ATOM 5583 C GLU 2322 17.000 32.296 45.314 1.00 41.26 ATOM 5583 C GLU 2322 20.782 28.777 47.973 1.00 41.26 ATOM 5585 N MSE 2323 20.687 27.561 46.103 1.00 39.61 ATOM 5586 CA MSE 2323 20.687 27.561 46.103 1.00 39.61 ATOM 5586 CA MSE 2323 20.538 26.319 46.848 1.00 37.88 ATOM 5587 CB MSE 2323 19.806 25.275 46.003 1.00 37.88 ATOM 5588 SC MSE 2323 19.806 25.275 46.003 1.00 35.05 ATOM 5589 SE MSE 2323 17.386 25.726 47.320 10.00 25.96 ATOM 5589 SE MSE 2323 17.386 25.726 47.320 10.00 25.96 ATOM 5590 CB MSE 2323 17.386 25.726 47.350 10.00 25.96 ATOM 5591 C MSE 2323 21.835 25.722 47.365 10.00 38.12 ATOM 5591 C MSE 2323 21.835 25.722 47.365 10.00 38.12 ATOM 5592 O MSE 2323 21.807 24.839 48.209 1.00 38.57 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 10.00 38.57 ATOM 5595 CB GLU 2324 22.976 26.195 46.822 10.00 38.57 ATOM 5596 CB GLU 2324 25.017 24.639 48.201 10.00 38.57 ATOM 5598 OEI GLU 2324 25.017 24.692 45.124 1.00 39.58 ATOM 5598 OEI GLU 2324 25.017 24.692 45.124 1.00 39.58 ATOM 5590 CC GLU 2324 26.830 25.638 44.216 1.00 40.09 ATOM 5590 CC GLU 2324 26.597 23.322 44.216 1.00 40.09 ATOM 5590 CC GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5590 CC GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5500 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.09 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.09 ATOM 5600 C GLU 2324 27.558 26.266 48.638 1.00 39.09 ATOM 5600 C GLU 2326 23.995 27.074 49.293 1.00 39.69 ATOM 5600 C GLU 2326 22.996 27.004 49.066 1.00 40.09 ATOM 5600 C GLU 2326 23.995 27.595 50.595 1.00 39.99 ATOM 5600 C GLU 2326 23.995 27.595 50.595 1.00 39.99 ATOM 5600 C GLU 2326 23.995 27.595 50.00 3.55 1.00 39.99 ATOM 5600 C GLU 2326 23.995 27.595 50.00 3.55 1.00 39		ATOM	5580	CD	GLU	2322		17.515		46.309	1.00 48.52
ATOM 5582 CG GLU 2322 20.785 28.713 46.749 1.00 49.57 ATOM 5584 C GLU 2322 20.785 28.713 46.749 1.00 41.07 ATOM 5585 N MSE 2323 20.687 27.561 46.103 1.00 41.07 ATOM 5585 CB MSE 2323 20.687 27.561 46.103 1.00 41.07 ATOM 5586 CA MSE 2323 20.687 27.561 46.103 1.00 49.57 ATOM 5586 CB MSE 2323 19.806 25.275 46.003 1.00 37.88 ATOM 5587 CB MSE 2323 19.806 25.275 46.003 1.00 37.88 ATOM 5589 CG MSE 2323 19.806 25.275 46.003 1.00 35.05 ATOM 5589 CC MSE 2323 17.386 25.726 47.320 1.00 25.63 ATOM 5580 CE MSE 2323 17.386 25.726 47.320 1.00 25.63 ATOM 5590 CE MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5590 C MSE 2323 21.835 25.722 47.365 1.00 38.12 ATOM 5593 N GLU 2324 22.976 26.195 46.882 1.00 38.50 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 1.00 38.54 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 1.00 38.94 ATOM 5597 CD GLU 2324 25.285 25.663 46.253 1.00 39.94 ATOM 5599 OEI GLU 2324 26.813 25.503 47.352 1.00 39.58 ATOM 5590 OEI GLU 2324 26.813 25.503 47.70 1.00 40.77 ATOM 5590 OEI GLU 2324 26.813 25.503 47.70 1.00 40.77 ATOM 5590 OEI GLU 2324 26.813 25.503 47.70 1.00 40.77 ATOM 5590 OEI GLU 2324 26.813 25.503 47.70 1.00 39.58 ATOM 5601 O GLU 2324 22.856 26.666 48.638 1.00 39.79 ATOM 5601 O GLU 2324 22.8580 26.015 49.046 1.00 49.79 ATOM 5601 O GLU 2324 22.8580 26.015 49.046 1.00 39.79 ATOM 5601 O GLU 2324 22.8580 26.015 49.046 1.00 39.79 ATOM 5601 O GLU 2324 25.800 26.015 49.046 1.00 39.79 ATOM 5601 CR VAL 2325 23.336 27.074 49.293 1.00 39.69 ATOM 5601 CR VAL 2325 23.356 27.074 49.293 1.00 39.69 ATOM 5601 CR VAL 2325 23.356 27.074 49.293 1.00 39.69 ATOM 5601 CR VAL 2325 23.356 27.075 40.00 39.79 ATOM 5602 CR VAL 2325 23.366 27.075 49.046 1.00 49.79 ATOM 5603 CR VAL 2325 22.054 28.125 51.068 1.00 40.93 ATOM 5604 CR VAL 2325 22.054 28.125 51.068 1.00 40.93 ATOM 5606 CC VAL 2325 22.054 28.125 51.068 1.00 40.93 ATOM 5607 C VAL 2325 22.054 28.125 51.068 1.00 40.93 ATOM 5608 CR VAL 2325 22.054 28.125 51.068 1.00 40.93 ATOM 5608 CR VAL 2325 22.054 28.125 51.068		ATOM	5581	OE1	GLU	2322		17.261	32.034	47.503	
ATOM 5583 C GLU 2322 20.782 28.777 47.973 1.00 41.07 41.26 ATOM 5586 N MSE 2323 20.687 27.561 46.103 1.00 39.61 ATOM 5586 CA MSE 2323 20.538 26.319 46.848 1.00 39.61 ATOM 5586 CG MSE 2323 19.806 25.275 46.003 1.00 39.61 ATOM 5589 SE MSE 2323 19.806 25.275 46.003 1.00 35.65 ATOM 5589 SE MSE 2323 17.336 25.752 47.320 1.00 25.96 ATOM 5589 SE MSE 2323 17.336 25.752 47.320 1.00 25.96 ATOM 5593 N MSE 2323 17.336 25.752 47.320 1.00 25.96 ATOM 5593 N MSE 2323 17.336 25.726 47.365 1.00 38.12 ATOM 5591 C MSE 2323 21.835 25.722 47.365 1.00 38.12 ATOM 5593 N MSE 2323 21.835 25.722 47.365 1.00 38.12 ATOM 5593 N MSE 2323 21.835 25.722 47.365 1.00 38.57 ATOM 5595 CG GLU 2324 22.976 26.195 46.882 1.00 38.57 ATOM 5595 CG GLU 2324 22.976 26.195 46.882 1.00 38.57 ATOM 5595 CG GLU 2324 25.017 24.692 44.216 1.00 39.03 ATOM 5595 CG GLU 2324 25.017 24.692 44.216 1.00 39.03 ATOM 5595 CG GLU 2324 25.017 24.692 44.216 1.00 39.03 ATOM 5595 CG GLU 2324 26.830 25.633 44.216 1.00 39.03 ATOM 5590 CE GLU 2324 26.830 25.633 43.770 1.00 40.79 ATOM 5590 CE GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5500 C GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.03 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 24.755 26.266 48.638 1.00 39.29 ATOM 5600 C GLU 2324 24.755 26.266 48.638 1.00 39.29 ATOM 5600 C GLU 2324 24.755 26.266 48.638 1.00 39.29 ATOM 5600 C GLU 2324 24.755 26.266 48.638 1.00 39.29 ATOM 5600 C GLU 2324 24.755 26.266 48.638 1.00 39.49 ATOM 5600 C GLU 2324 24.755 26.266 48.638 1.00 39.49 ATOM 5600 C GLU 2326 23.955 27.074 49.293 1.00 39.69 ATOM 5600 C GLU 2326 23.955 27.074 49.293 1.00 39.69 ATOM 5600 C GLU 2326 23.955 27.074 49.293 1.00 39.69 ATOM 5600 C GLU 2326 23.955 27.095 50.552 1.00 40.00 39.79 ATOM 5600 C GLU 2326 23.955 27.095 50.552 1.00 40.00 39.79 ATOM 5600 C GLU 2326 23.955 27.095 50.552 1.00 34.39 3		MOTA	5582	OE2	GLU	2322		17.000	32.296	45.314	
ATOM 5585 N MSE 2323 20.687 27.561 46.103 1.00 37.861		MOTA	5583	С	GLU			20.785	28.713	46.749	
ATOM 5586 CA MSE 2323 20.538 26.319 46.848 1.00 37.88 ATOM 5588 CB MSE 2323 19.806 25.275 46.003 1.00 35.05 37.88 ATOM 5589 CB MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5590 CB MSE 2323 21.807 24.839 48.209 1.00 26.31 ATOM 5591 C MSE 2323 21.807 24.839 48.209 1.00 26.31 ATOM 5593 N GLU 2324 22.976 26.195 46.882 1.00 38.50 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 1.00 38.57 47.365 47.365 1.00 38.57 47.365 47.365 1.00 38.57 47.365 47.365 1.00 38.57 47.365 47.365 1.00 38.57 47.365 47.365 47.365 1.00 39.03 47.365 47.365 47.365 1.00 39.03 47.365 47.36	10			0				20.782	28.777	47.973	1.00 41.26
ATOM 5587 CB MSE 2323 19.806 25.275 46.003 1.00 35.05 1.00		ATOM			MSE			20.687	27.561	46.103	1.00 39.61
ATOM 5588 CG MSE 2323 18.309 25.537 45.788 1.00 30.55 ATOM 5590 CE MSE 2323 17.386 25.726 47.327 1.00 25.96 ATOM 5591 C MSE 2323 21.838 25.722 47.365 1.00 38.12 ATOM 5592 C MSE 2323 21.837 24.839 48.209 1.00 38.50 ATOM 5593 N GLU 2324 22.976 26.195 46.882 1.00 38.50 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 1.00 38.51 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 1.00 39.03 ATOM 5595 CB GLU 2324 25.285 25.683 47.352 1.00 38.94 ATOM 5595 CB GLU 2324 25.285 25.683 46.253 1.00 39.03 ATOM 5595 CB GLU 2324 26.230 24.489 44.216 1.00 40.09 ATOM 5599 OE2 GLU 2324 26.813 25.503 43.770 1.00 40.77 ATOM 5590 OE2 GLU 2324 26.813 25.503 43.770 1.00 40.77 ATOM 5500 C GLU 2324 26.813 25.503 43.770 1.00 40.77 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5600 C GLU 2324 26.813 25.503 49.734 1.00 39.99 ATOM 5600 C GLU 2324 26.813 25.503 49.734 1.00 39.99 ATOM 5600 C GLU 2324 26.813 27.074 49.293 1.00 39.43 ATOM 5600 C GLU 2324 26.813 27.074 49.293 1.00 39.49 ATOM 5600 C WAL 2325 23.936 27.074 49.293 1.00 39.49 ATOM 5600 C WAL 2325 22.031 27.074 49.293 1.00 39.49 ATOM 5600 C WAL 2325 22.031 27.074 49.293 1.00 39.49 ATOM 5600 C WAL 2325 23.936 27.074 49.293 1.00 39.49 ATOM 5600 C WAL 2325 22.031 27.074 49.293 1.00 39.49 ATOM 5600 C WAL 2325 22.031 27.075 49.046 1.00 40.22 ATOM 5601 CB WAL 2325 22.032 23.935 27.074 49.293 1.00 39.49 ATOM 5601 CB WAL 2325 22.032 23.935 27.075 20.035 20.035 20.035 ATOM 5601 CB LEU 2326 23.395 27.855 51.487 1				CA	MSE				26.319	46.848	1.00 37.88
ATOM 5589 SE MSE 2323 17.386 25.726 47.320 1.00 25.96				CB	MSE			19.806	25.275	46.003	1.00 35.05
ATOM 5590 CE MSE 2323 17.938 24.311 48.279 1.00 26.31 ATOM 5591 C MSE 2323 21.835 25.722 47.365 1.00 38.12 ATOM 5592 O MSE 2323 21.835 25.722 47.365 1.00 38.12 ATOM 5593 N GLU 2324 22.976 26.195 46.882 1.00 38.57 ATOM 5595 CB GLU 2324 22.976 26.195 46.882 1.00 38.57 ATOM 5595 CB GLU 2324 22.976 25.636 47.352 1.00 38.94 ATOM 5595 CB GLU 2324 25.285 25.636 47.352 1.00 39.03 ATOM 5595 CB GLU 2324 25.285 25.636 47.352 1.00 39.03 ATOM 5596 CG GLU 2324 25.017 24.692 45.124 1.00 39.03 ATOM 5598 OE1 GLU 2324 26.530 24.489 44.216 1.00 40.79 ATOM 5598 OE1 GLU 2324 26.813 25.503 43.770 1.00 40.77 ATOM 5598 OE2 GLU 2324 26.813 25.503 43.770 1.00 40.77 ATOM 5600 C GLU 2324 26.813 25.503 43.770 1.00 40.77 ATOM 5600 C GLU 2324 26.895 26.266 48.638 1.00 39.29 ATOM 5600 C GLU 2324 26.895 26.266 48.638 1.00 39.29 ATOM 5600 C GLU 2324 25.880 26.015 49.046 1.00 39.79 ATOM 5601 C GLU 2324 25.880 26.015 49.046 1.00 39.79 ATOM 5603 CA VAL 2325 23.936 27.074 49.293 1.00 39.49 ATOM 5603 CA VAL 2325 24.351 27.668 50.552 1.00 40.62 ATOM 5605 CGI VAL 2325 24.061 30.036 49.750 1.00 40.62 ATOM 5605 CGI VAL 2325 24.061 30.036 49.750 1.00 40.63 ATOM 5605 CGI VAL 2325 25.553 29.545 51.487 1.00 40.30 ATOM 5605 CGI VAL 2325 25.553 29.545 51.487 1.00 39.49 ATOM 5605 CGI VAL 2325 25.553 29.545 51.487 1.00 39.79 ATOM 5605 CGI VAL 2325 22.5553 29.545 51.487 1.00 39.79 ATOM 5607 C VAL 2325 22.5553 29.545 51.487 1.00 39.79 ATOM 5608 O VAL 2325 22.5553 29.545 51.487 1.00 39.79 ATOM 5608 O VAL 2325 22.5553 29.545 51.487 1.00 39.79 ATOM 5608 CGI VAL 2326 22.342 27.716 53.769 1.00 39.40 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.40 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.40 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.64 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.64 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.64 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.64 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.64 ATOM 5610 CA LEU 2328 22.340 32.500 55.299 1.00 39.64 ATOM 5620 CB HIS 2327 22.002 29.811 50.00 37.									25.537	45.788	1.00 30.55
ATOM 5591 C MSE 2323 21.835 25.722 47.365 1.00 38.50 ATOM 5592 O MSE 2323 21.807 24.839 48.209 1.00 38.50 ATOM 5593 N GLU 2324 22.976 26.195 46.882 1.00 38.57 ATOM 5595 CB GLU 2324 22.2076 26.195 46.882 1.00 38.57 ATOM 5595 CB GLU 2324 25.285 25.683 46.253 1.00 39.03 ATOM 5596 CG GLU 2324 25.017 24.692 45.124 1.00 39.58 ATOM 5597 CD GLU 2324 26.230 24.489 44.216 1.00 40.09 ATOM 5598 OE1 GLU 2324 26.630 24.489 44.216 1.00 40.09 ATOM 5599 OE2 GLU 2324 26.597 23.322 43.943 1.00 39.58 ATOM 5599 OE2 GLU 2324 26.597 23.322 43.943 1.00 39.49 ATOM 5601 C GLU 2324 26.597 23.322 43.943 1.00 39.92 ATOM 5602 N VAL 2325 23.880 26.015 49.046 1.00 39.79 ATOM 5603 CA VAL 2325 22.880 26.015 49.046 1.00 39.99 ATOM 5604 CB VAL 2325 22.8936 27.074 49.293 1.00 39.99 ATOM 5606 CG2 VAL 2325 22.303 29.039 50.355 1.00 40.22 ATOM 5606 CG2 VAL 2325 22.5533 29.039 50.355 1.00 40.22 ATOM 5608 CG2 VAL 2325 22.5553 29.545 51.686 1.00 40.30 ATOM 5608 O VAL 2325 22.5553 27.568 51.00 40.22 ATOM 5609 N LEU 2326 23.163 27.868 51.00 40.27 ATOM 5600 CG2 VAL 2325 23.163 27.868 51.00 40.27 ATOM 5608 CG2 VAL 2325 23.163 27.868 51.00 40.27 ATOM 5608 CG2 VAL 2325 23.163 27.868 51.00 40.27 ATOM 5608 CG2 VAL 2325 23.163 27.865 51.686 1.00 40.30 ATOM 5608 O VAL 2325 22.054 88.125 51.00 40.27 ATOM 5608 O VAL 2325 22.054 88.125 51.00 40.27 ATOM 5608 O VAL 2325 22.054 88.125 51.00 40.27 ATOM 5610 CA LEU 2326 22.054 88.125 51.00 39.99 ATOM 5610 CA LEU 2326 22.054 88.125 51.00 39.99 ATOM 5610 CA LEU 2326 22.054 88.125 51.00 39.30 ATOM 5610 CB LEU 2326 22.054 88.125 51.00 39.30 ATOM 5610 CB LEU 2326 22.054 88.125 51.00 39.30 ATOM 5610 CB LEU 2326 22.054 88.125 51.00 39.30 ATOM 5610 CB LEU 2326 22.054 88.125 51.00 39.60 ATOM 5610 CB LEU 2326 22.054 88.125 51.00 39.60 ATOM 5610 CB LEU 2326 22.054 89.00 55.396 1.00 37.59 ATOM 5610 CB LEU 2326 22.054 89.00 55.396 1.00 37.59 ATOM 5610 CB LEU 2326 22.054 89.00 55.396 1.00 37.87 ATOM 5610 CD LEU 2326 22.054 39.00 55.255 1.00 39.30 ATOM 5610 CB LEU 2326 22.054 39.00 55.255 1.00 39.3	15							17.386		47.320	1.00 25.96
ATOM 5592 O MSE 2323 ATOM 5593 N GLU 2324 22.976 26.195 46.882 1.00 38.57 ATOM 5594 CA GLU 2324 22.976 26.195 46.882 1.00 38.94 ATOM 5595 CB GLU 2324 25.285 25.683 46.253 1.00 38.94 ATOM 5596 CG GLU 2324 25.285 25.683 46.253 1.00 39.58 ATOM 5597 CC GLU 2324 25.285 25.683 46.253 1.00 39.58 ATOM 5598 OEI GLU 2324 26.230 24.489 44.216 1.00 40.09 ATOM 5599 OEZ GLU 2324 26.597 23.322 43.943 1.00 39.43 ATOM 5500 C GLU 2324 26.597 23.322 43.943 1.00 39.49 ATOM 5600 C GLU 2324 26.597 23.322 43.943 1.00 39.49 ATOM 5601 O GLU 2324 26.597 23.322 43.943 1.00 39.49 ATOM 5602 C GLU 2324 26.597 23.322 43.943 1.00 39.49 ATOM 5603 CA VAL 2325 23.936 27.074 49.293 1.00 39.49 ATOM 5604 CB VAL 2325 24.051 27.074 49.293 1.00 39.49 ATOM 5605 CGI VAL 2325 24.051 30.036 49.750 1.00 40.62 ATOM 5606 CG2 VAL 2325 24.061 30.036 49.750 1.00 40.22 ATOM 5607 C VAL 2325 25.553 29.545 51.666 1.00 40.30 ATOM 5608 C VAL 2325 23.553 27.825 51.487 1.00 39.79 ATOM 5608 C VAL 2325 23.163 27.825 51.487 1.00 39.79 ATOM 5609 N LEU 2326 22.342 27.716 53.769 1.00 39.49 ATOM 5610 CA LEU 2326 22.342 27.716 53.769 1.00 39.40 ATOM 5610 CA LEU 2326 22.081 26.375 55.666 1.00 37.59 ATOM 5610 CA LEU 2326 22.081 26.375 55.666 1.00 37.59 ATOM 5610 CA LEU 2326 22.081 26.375 55.566 1.00 37.59 ATOM 5610 CA LEU 2326 22.081 26.375 55.566 1.00 37.59 ATOM 5610 CB LEU 2326 22.081 26.375 55.666 1.00 37.59 ATOM 5610 CB LEU 2326 22.081 26.375 55.566 1.00 37.59 ATOM 5610 CB LEU 2326 22.081 26.375 55.566 1.00 39.69 ATOM 5610 CB LEU 2326 22.081 26.375 55.566 1.00 39.69 ATOM 5610 CB LEU 2326 22.081 26.375 55.666 1.00 37.87 ATOM 5610 CB LEU 2326 22.081 26.375 55.666 1.00 37.87 ATOM 5610 CB LEU 2326 22.081 25.000 56.287 1.00 39.69 ATOM 5610 CB LEU 2326 22.081 25.000 56.287 1.00 39.69 ATOM 5610 CB LEU 2326 22.081 25.000 56.287 1.00 39.69 ATOM 5610 CB LEU 2326 22.081 25.000 56.287 1.00 39.69 ATOM 5610 CB LEU 2326 22.081 25.000 56.287 1.00 39.69 ATOM 5620 CB LEU 2328 22.081 25.000 57.99 50.00 39.81 ATOM 5621 CD2 LEU 2328 22.081 25.000 56.287 1.00 37.87 ATOM 5622 CD2 LEU 2328 22.081 2							:	17.938		48.279	
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40 ATOM 5614 CD2 LEU 2326 21.063 25.000 56.287 1.00 32.79 ATOM 5615 C LEU 2326 22.797 28.755 54.783 1.00 39.66 ATOM 5616 O LEU 2326 23.851 28.600 55.396 1.00 39.64 ATOM 5617 N HIS 2327 22.002 29.811 54.946 1.00 40.11 ATOM 5618 CA HIS 2327 22.012 32.250 55.239 1.00 39.31 ATOM 5620 CG HIS 2327 22.012 32.250 55.239 1.00 39.31 ATOM 5621 CD2 HIS 2327 22.840 32.560 54.035 1.00 38.31 ATOM 5622 ND1 HIS 2327 22.562 32.464 52.713 1.00 37.82 ATOM 5623 CEI HIS 2327 24.149 32.987 54.122 1.00 38.78 ATOM 5623 CEI HIS 2327 24.643 33.136 52.905 1.00 37.87 ATOM 5625 C HIS 2327 24.643 33.136 52.905 1.00 37.87 ATOM 5625 C HIS 2327 21.544 30.791 57.183 1.00 41.82 ATOM 5626 O HIS 2327 20.319 30.621 57.187 1.00 42.05 ATOM 5628 CA LEU 2328 22.267 30.898 58.291 1.00 42.60 ATOM 5630 CG LEU 2328 22.167 29.657 60.402 1.00 42.78 ATOM 5630 CG LEU 2328 22.167 29.657 60.402 1.00 42.78 ATOM 5631 CD1 LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5633 C LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5633 C LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5633 C LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5633 C LEU 2328 22.382 22.151 60.298 1.00 45.00 60 ATOM 5634 O LEU 2328 23.271 32.422 60.448 1.00 45.19 ATOM 5635 N ARG 2329 21.104 32.947 60.711 1.00 46.79		MOTA	5612	CG	LEU	2326	2	21.116		55.666	1.00 35.15
ATOM 5615 C LEU 2326 22.797 28.755 54.783 1.00 39.66 ATOM 5616 O LEU 2326 23.851 28.600 55.396 1.00 39.64 ATOM 5617 N HIS 2327 22.002 29.811 54.946 1.00 40.11 ATOM 5618 CA HIS 2327 22.319 30.892 55.875 1.00 40.64 45 ATOM 5619 CB HIS 2327 22.012 32.250 55.239 1.00 39.31 ATOM 5620 CG HIS 2327 22.840 32.560 54.035 1.00 38.31 ATOM 5621 CD2 HIS 2327 22.840 32.560 54.035 1.00 38.31 ATOM 5622 ND1 HIS 2327 24.149 32.987 54.122 1.00 38.78 ATOM 5623 CE1 HIS 2327 24.643 33.136 52.905 1.00 37.87 ATOM 5624 NE2 HIS 2327 24.643 33.136 52.905 1.00 37.87 ATOM 5626 O HIS 2327 23.700 32.824 52.032 1.00 37.87 ATOM 5625 C HIS 2327 21.544 30.791 57.183 1.00 41.82 ATOM 5626 O HIS 2327 20.319 30.621 57.187 1.00 42.05 ATOM 5628 CA LEU 2328 22.67 30.898 58.291 1.00 42.05 ATOM 5629 CB LEU 2328 21.661 30.861 59.612 1.00 42.78 ATOM 5630 CG LEU 2328 21.661 30.861 59.612 1.00 42.78 ATOM 5631 CD1 LEU 2328 22.167 29.657 60.402 1.00 42.78 ATOM 5632 CD2 LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5633 C LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5634 O LEU 2328 22.082 32.151 60.298 1.00 45.00 ATOM 5635 N ARG 2329 21.104 32.947 60.711 1.00 46.79		ATOM		CD1	LEU	2326	:	19.740	26.806	55.225	1.00 34.39
ATOM 5616 O LEU 2326 23.851 28.600 55.396 1.00 39.64 ATOM 5617 N HIS 2327 22.002 29.811 54.946 1.00 40.11 ATOM 5618 CA HIS 2327 22.319 30.892 55.875 1.00 40.64 45 ATOM 5619 CB HIS 2327 22.012 32.250 55.239 1.00 39.31 ATOM 5620 CG HIS 2327 22.840 32.560 54.035 1.00 38.31 ATOM 5621 CD2 HIS 2327 22.562 32.464 52.713 1.00 37.82 ATOM 5622 ND1 HIS 2327 24.149 32.987 54.122 1.00 38.78 ATOM 5623 CE1 HIS 2327 24.643 33.136 52.905 1.00 37.87 ATOM 5624 NE2 HIS 2327 24.643 33.136 52.905 1.00 37.87 ATOM 5625 C HIS 2327 23.700 32.824 52.032 1.00 37.87 ATOM 5626 O HIS 2327 21.544 30.791 57.183 1.00 41.82 ATOM 5626 O HIS 2327 20.319 30.621 57.187 1.00 42.05 ATOM 5627 N LEU 2328 22.267 30.898 58.291 1.00 42.60 ATOM 5628 CA LEU 2328 21.661 30.861 59.612 1.00 43.72 55 ATOM 5629 CB LEU 2328 22.167 29.657 60.402 1.00 42.78 ATOM 5631 CD1 LEU 2328 22.167 29.657 60.402 1.00 42.78 ATOM 5632 CD2 LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5633 C LEU 2328 22.379 27.213 60.770 1.00 40.90 ATOM 5634 O LEU 2328 22.380 28.111 59.590 1.00 40.44 ATOM 5633 C LEU 2328 22.082 32.151 60.298 1.00 45.00 60 ATOM 5634 O LEU 2328 23.271 32.422 60.448 1.00 45.19 ATOM 5635 N ARG 2329 21.104 32.947 60.711 1.00 46.79	40			CD2							1.00.32.79
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                   CB
                        ARG
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                                                  35.294
                                                           60.699
                                                                    1.00 49.55
                              2329
     ATOM
             5638
                   CG
                        ARG
                                         20.906
                                                  35.568
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     ATOM
             5639
                        ARG
                              2329
                                         22.219
                                                  36.294
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                              2329
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                                         22.775
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     ATOM
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	MOTA	6011	N	HIS	3166		26.426	-8.943	13.331	1.00 39.	
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5	ATOM	6013	CB	HIS	3166		25.798	-6.594	12.888	1.00 40.	57
	ATOM	6014	CG	HIS	3166		25.774	-6.410	11.404	1.00 43.	
	ATOM	6015		HIS	3166		25.865	-5.289	10.648	1.00 44.	
	ATOM	6016		HIS	3166		25.566	-7.451	10.522	1.00 44.	
	ATOM	6017		HIS	3166		25.529	-6.979	9.286	1.00 45.	
10	ATOM	6018		HIS	3166		25.707	-5.669	9.334	1.00 45.	
	ATOM	6019	C	HIS	3166		27.108	-7.269	14.875	1.00 36.	
	ATOM	6020	ō	HIS	3166		26.167	-7.230	15.669	1.00 35.	
	ATOM	6021	N	ALA	3167		28.365	-7.097	15.255	1.00 34.	
	ATOM	6022	CA	ALA	3167		28.677	-6.791	16.644	1.00 32.	
15	ATOM	6023	CB	ALA	3167		29.688	-7.777	17.200	1.00 32.	
	ATOM	6024	C	ALA	3167		29.239	-5.384	16.648	1.00 32.	
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	ATOM	6026	N	VAL	3168		28.704	-4.542	17.526	1.00 31.	
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20	ATOM	6028	CB	VAL	3168		28.226	-2.278	16.685	1.00 27.	
	ATOM	6029	CG1		3168		28.195	-2.276	15.272	1.00 27.	
	ATOM '	6030	CG2		3168		26.811			1.00 26.	
	ATOM	6030	C	VAL	3168			2.239	17.239 19.018	1.00 26.	
	ATOM	6032	ŏ	VAL	3168		29.070 28.329			1.00 26.	
25	· ATOM	6033	N	PRO	3169		29.860	-3.136	19.847	1.00 26.	
	ATOM	6033	CD	PRO	3169		30.703	-1.571	19.322	1.00 25.	
	ATOM	6035		PRO	3169			-0.764	18.434	1.00 26.	
	ATOM	6036	CA	•	3169		29.841	-0.990	20.663	1.00 25.	
	ATOM	6037	CB CG	PRO			31.012	-0.015	20.660	1.00 25.	
30		6038		PRO	3169		31.725	-0.253	19.382	1.00 26.	
50	MOTA		C	PRO	3169		28.531	-0.213	20.730	1.00 26.	
•	MOTA	6039	0	PRO	3169		27.948	0.107	19.693	1.00 25.	
•	MOTA	6040	N	ALA	3170		28.074	0.102	21.933	1.00 26.	
	MOTA	6041	CA	ALA	3170		26.832	0.862	22.088	1.00 26.	
35	MOTA	6042	CB	ALA	3170		26.484	1.017	23.564	1.00 26.	
55	ATOM	6043	C	ALA	3170		26.983	2.235	21.454	1.00 26.	
	ATOM	6044 6045	0	ALA	3170		28.101	2.734	21.307	1.00 27.	
•	ATOM		N	ALA	3171		25.854	2.818	21.058	1.00 26.	
	ATOM	6046	CA	ALA			25.790	4.148	20.450	1.00 26.	
40	ATOM	. 5047	CB	ALA	3171		26.711	5.116	21.181	1.00 26.	
40	MOTA	6048	Ç	ALA	3171		26.087	4.202	18.963	1.00 27.	
	MOTA	6049	0	ALA	3171		25.857	5.226	18.312	1.00 28.	
	MOTA	6050	N	LYS	3172		26.599	3.115	18.412	1.00 28.	
	MOTA	6051	CA	LYS	3172		26.906	3.097	16.995	1.00 29.	
45	MOTA	6052	CB	LYS	3172		27.845	1.923	16.696	.1.00 30.	
43	ATOM	6053	CG	LYS	3172		28.457	1.956	15.304	1.00 32.	_
	ATOM	6054	CD	LYS	3172		29.358	0.753	15.044	1.00 33.	
	ATOM	6055	CE	LYS	3172		30.144	0.941	13.746	1.00 34.	
	ATOM	6056	NZ	LYS	3172		29.263	1.283	12.577	1.00 35.	_
50	MOTA	6057	C	LYS	3172		25.624	2.987	16.159	1.00 29.	
30	ATOM	6058	0	LYS	3172		24.585	2.528	16.647	1.00 29.3	22
	ATOM	6059	N	THR	3173		25.690	3.432	14.909	1.00 28.	75
	MOTA	6060	CA	THR	3173		24.535	3.338	14.033	1.00 28.0	80
	MOTA	6061	CB	THR	3173		24.457	4.545	13.109	1.00 28.3	30
	ATOM	6062		THR	3173		23.941	5.653	13.857	1.00 27.	79
5 <i>5</i>	MOTA	6063		THR	3173		23.543	4.260	11.928	1.00 28.8	33
	MOTA	6064	С	THR	3173	2	24.645	2.032	13.258	1.00 29.4	
	MOTA	6065	0	THR	3173	2	25.713	1.681	12.755	1.00 30.2	
	MOTA	6066	. N	VAL	3174	2	23.548	1.291	13.197	1.00 29.8	
	ATOM	6067	CA	VAL	3174		23.557	0.008	12.510	1.00 30.0	
60	ATOM	6068	CB	VAL	3174		23.186	-1.124	13.484	1.00 28.8	
		6069	CG1	VAL	3174		22.983	-2.428	12.740	1.00 28.0	
	ATOM	6070	CG2	VAL	3174		24.293	-1.283	14.500	1.00 28.8	

	ATOM ATOM	6071 6072	C O	VAL VAL	3174 3174		22.619 21.512	0.013 0.549		1.00 30.91 1.00 30.79
	ATOM	6073	N	LYS	3175		23.076	-0.578		1.00 32.06
_	ATOM	6074	CA	LYS	3175		22.267	-0.628	9.024	1.00 33.55
5	ATOM	6075	CB	LYS	3175		22.770	0.408		1.00 34.53
	ATOM	6076	CG	LYS	3175		21.870	0.577		1.00 36.89
	ATOM	6077	CD	LYS	3175		22.337	1.726		1.00 39.24
	ATOM ATOM	6078 6079	CE NZ	LYS LYS	3175 3175		21.393 21.784	1.951 3.133		1.00 39.73
10	ATOM	6080	C	LYS	3175		22.249	-2.024		1.00 41.45 1.00 33.32
	ATOM	6081	ŏ	LYS	3175		23.286	-2.601		1.00 33.32
	ATOM	6082	N	PHE	3176		21.050	-2.558		1.00 33.70
	MOTA	6083	CA	PHE	3176		20.865	-3.873		1.00 34.13
	ATOM	6084	CB	PHE	3176		19.968	-4.721		1.00 31.96
15	MOTA	6085	CG	PHE	3176		20.587	-5.082	9.845	1.00 30.12
	· ATOM	6086		PHE	3176	•	21.910	-5.497	9.906	1.00 29.71
	MOTA	6087		PHE	3176		19.838	-5.071	11.005	1.00 29.63
	ATOM ATOM	6088 6089		PHE	3176		22.478	-5.904	11.102	1.00 29.50
20	ATOM	6090	CEZ	PHE	3176 3176		20.399 21.727	-5.476		1.00 30.45
	ATOM	· 6091	C	PHE	3176		20.197	-5.896 -3.704	.12.25.7 6.300	1.00 29.17 1.00 35.61
	ATOM	6092	ŏ	PHE	3176		19.304	-2.867	6.147	1.00 35.61 1.00 36.07
	ATOM	6093	N	LYS	3177		20.625	-4.483	5.315	1.00 36.95
	ATOM	6094	CA	LYS	3177		20.002	-4.383	4.014	1.00 38.56
25	ATOM	6095	СВ	LYS	3177		20.748	-3.380	3.125	1.00 39.62
,	ATOM	6096	CG	LYS	3177		22.254	-3.523		1.00-41.82
	ATOM	6097	CD	LYS	3177	•	22.844	-2.304	2.342	1.00 42.64
•	MOTA MOTA	6098	CE	LYS	3177	٠.	24.365	-2.276	2.402	1.00 44.37
30	ATOM	6099 6100	NZ C	LYS	3177 3177		24.905	-1.054	1.707	1.00 45.40
.	ATOM	6101	Ö	LYS	3177		19.841 20.598	-5.721 -6.657	3.322 3.551	1.00 38.93 1.00 37.98
•	ATOM	6102	Ñ	CYS	3178		18.806	-5.799	2,498	1.00 37.98 1.00 40.12
٠.	ATOM	6103	CA	CYS	3178		18.495	-6:999	1.748	1.00 41.37
	MOTA	6104	CB	CYS	3178		17.349	-7.739	2.427	1.00 42.64
35	· ATOM	6105	SG	CYS	3178		17.858	-8.494	3.970	1.00 44.96
•	ATOM	6106	С	CYS	3178		18.112	-6.600	0.335	1.00 41.53
	MOTA	6107	0	CYS	3178	• •	16.950	-6.693	-0.061	1.00 41.06
_	ATOM ATOM	6108 6109	N	PRO	3179		19.095	-6.122	-0.438	1.00 42.05
40	MOTA	6110	· CD	PRO PRO	3179 3179		20.524 18.842	-6.009	-0.099	1.00 41.96
	ATOM	6111	СВ	PRO	3179		20.218	-5.706 -5.259	-1.816 -2.297	
	ATOM	6112	CG	PRO	3179		21.167	-6.059	-2.237	1.00 42.84 1.00 42.62
	ATOM	6113	C	PRO	3179		18.252	-6.840	-2.645	1.00 43.20
	ATOM	6114	. 0	PRO	3179		18:834	-7.924	-2.760	1.00 42.85
45	MOTA	6115	N	SER	3180		17.070	-6.595	-3.193	1.00 43.70
	ATOM	6116	CA	SER	3180		16.421	-7.594	-4.010	1.00 45.13
	ATOM	6117	CB	SER	3180		15.563	-8.523	-3.142	1.00 45.23
•	MOTA MOTA	6118 6119	OG C	SER SER	3180 3180		14.694	-7.799	-2.301	1.00 45.85
50	ATOM	6120	Ö	SER			15.589	-6.957	-5.109	1.00 45.73
	ATOM	6121	N	SER	3180		15.593 14.892	-5.737 -7.796	-5.290 -5.861	1.00 45.62 1.00 46.63
	ATOM	6122	CA	SER	3181		14.068	-7.312	-6.947	1.00 45.65
	ATOM	6123	CB	SER	3181		14.935	-7.013	-8.163	1.00 47.39
	MOTA	6124	OG	SER	3181		14.141	-6.509	-9.217	1.00 48.09
55	MOTA	6125	С	SER	3181		13.012	-8.337	-7.317	1.00 48.28
	MOTA	6126	0	SER	3181	•	12.908	-9.396	-6.700	1.00 48.27
	ATOM	6127	N	GLY	3182		12.233	-8.010	-8.338	1.00 49.22
	ATOM	6128	CA	GLY	3182	•	11.183	-8.897	-8.788	1.00 49.41
60	ATOM ATOM	6129 6130	C	GLY	3182		10.032	-8.069	-9.310	1.00 49.66
. 0	ATOM	6131	O N	GLY THR	3182 3183		9.958	-6.870	-9.055	1.00 49.58
	ATOM	6132	CA	THR	3183		9.132 7.995		-10.051 -10.580	1.00 49.75
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                                                     -4.478
55
     ATOM
              6249
                     CA
                         PHE
                                3197
                                            8.844
                                                               14.560
                                                                        1.00 40.76
                                                                        1.00 39.76
1.00 38.89
     ATOM
              6250
                     CB
                          PHE
                                3197
                                            10.252
                                                     -4.686
                                                               13.984
                                                     -3.881
     ATOM
              6251
                          PHE
                                3197
                                            11.335
                     CG
                                                               14.662
      ATOM
              6252
                     CD1 PHE
                                3197
                                            11.335
                                                     -3.688
                                                               16.043
                                                                        1.00 38.85
                                3197
                                            12.385
                                                     -3.347
      ATOM'
              6253
                     CD2 PHE
                                                               13.914
                                                                        1.00 38.27
60
     MOTA
              6254
                     CE1 PHE
                                3197
                                            12.366
                                                     -2.973
                                                               16.672
                                                                        1.00 37.34
      MOTA
              6255
                     CE2 PHE
                                3197
                                            13.424
                                                     -2.630
                                                               14.536
                                                                       1.00 38.68
                               3197
                                           13.409
     ATOM
                     CZ
              6256
                         PHE
                                                     -2.444
                                                               15.919
                                                                        1.00.37.81
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	ATOM ATOM ATOM	6257 6258 6259	0	PHE PHE LYS	3197	8.294 8.190 7.918	-3.108 -2.776		1.00	40.60
5	ATOM ATOM ATOM	6260 6261 6262	CA CB	LYS LYS	3198 3198	7.390 6.026	-2.321 -0.982 -0.787	15.181 14.934 15.609	1.00	41.31 42.03 43.37
	ATOM ATOM	6263 6264	CD CE	LYS LYS	3198 3198	4.866 3.558 2.467	-1.536 -1.226 -2.238	14.974 15.704 15.356	1.00	44.87 46.03 46.93
10	ATOM ATOM ATOM	6265 6266 6267		LYS LYS	3198 3198 3198	1.198 8.353 8.953	-1.998 0.055 -0.142	16.109 15.483 16.535	1.00	47.00 41.33 41.31
	ATOM ATOM ATOM	6268 6269 6270	N CD	PRO PRO	3 <u>199</u> 3199	8.505 7.770	1.181 1.579	14.778 13.571	1.00 1.00	40.99
15	ATOM ATOM	6271 6272	CA CB CG	PRO PRO PRO	3199 3199 3199	9.407 9.091 7.713	2.251 3.393 3.071	15.210 14.240 13.739	1.00	40.86 41.01 41.45
	ATOM ATOM ATOM	6273 6274 6275	C O .N	PRO PRO ASP	3199 3199 3200	9.250 10.213 8.053	2.647 3.048 2.523	16.673 17.311 17.226	1.00 1.00	40.59 40.53
20	MOTA MOTA	6276 6277	CA CB	ASP ASP	3200 3200	7.914 6.474	2.886	18.626	1400	41.07 :41.63 43.48
	ATOM ATOM ATOM	6278 6279 6280	CG OD1 OD2	ASP ASP ASP	3200 3200 3200	6.150 5.880 6.203	4.673 4.927 5.550	18.575 17.375 19.463	1.00	46.03 47.86 47.33
25	ATOM ATOM ATOM	6281 6282 6283	CO	ASP ASP	3200 3200	8.465 8.395	1.849 2.021	19.591 20.807	1.00	40.73
	ATCM ATOM	6284 6285	N CA CB	HIS HIS	3201 3201 3201	9.040 9.625 9.797	0.782 -0.239 -1.562	19.052 19.906 19.167	1.00 1.00 1.00	39.26
30	ATOM ATOM ATOM	6286 6287 6288	CD2	HIS HIS	3201 3201 3201	8.508 8.210 7.329	-2.254 -3.247	18.868 17.999	1.00	40.22 39.97
25	MOTA MOTA	6289 6290	CE1 NE2	HIS HIS	3201 3201	6.358 6.867	-1.932 -2.695 -3.500	19.505 19.036 18.121	1.00	40.01 40.19 40.73
35	ATOM ATOM ATOM	6291 6292 6293	C . O N	HIS HIS ARG	3201 3201 3202	10.978 11.534 11.523	0.192 -0.475 1.290	20.465 21.333 19.957	1.00 1.00	39.03 38.04
40	ATOM ATOM	6294 6295	CA CB	ARG ARG	3202 3202	12.788 13.979	1.775 1.192	20.478	1.00	38.42 37.66 37.22
70	ATOM ATOM ATOM	6296 .6297 6298	CG CD NE	ARG ARG ARG	3202 3202 3202	14.136 15.197 16.549	1.692 0.897 1.048	18.271 17.509 18.057	1.00	37.18 36.43 35.84
45	ATOM ATOM ATOM	6299 6300 6301		ARG ARG ARG	3202 3202	17.309 16.867	2.138	17.929 17.265	1.00 1.00	34.55 33.05
	ATOM ATOM	6302 6303	C	ARG ARG	3202 3202 3202	18.520 12.791 12.181	2.162 3.290 3.903	18.469 20.435 19.558	1.00 1.00 1.00	
50	ATOM ATOM ATOM	6304 6305 6306	N CA CB	ILE ILE	3203 3203 3203	13.453 13.547	3.891 5.333	21.412 21.486	1.00	38.58 39.83
	ATOM. ATOM	6307 6308	CG2 CG1	ILE	3203 3203	14.358 15.647 14.650	5.731 4.903 7.225	22.720 22.782 22.669	1.00 1.00	41.46
55	ATOM ATOM ATOM	6309 6310 6311	CD1 C O	ILE ILE ILE	3203 3203 3203	15.454 14.237 15.319	7.703 5.850	23.816 20.218	1.00	42.07 40.01
	ATOM ATOM	6312 6313	N CA	GLY GLY	3204 3204	13.609 14.187	5.391 6.805 7.325	19.857 19.544 18.317	1.00 : 1.00 :	40.57 40.51
60	ATOM ATOM ATOM	6314 6315 6316		GLY GLY	3204 3204 3205	13.725 13.913 13.116	6.535 6.958 5.380	17.098 15.956 17.345	1.00 4	40.21 39.93
	ATOM ATOM	6317 6318	CA	GLY GLY	3205 3205	12.635 13.723	4.553	16.259 15.296	1.00 d 1.00 d 1.00 d	39.84

	ATOM.	6319	_	CTV	3205		14 007	4 051	15 652	1 00 0	
	ATOM.	6320	N O	GLY TYR	3205		14.897 13.320	4.051	15.657	1.00 3	
	ATOM	6321	CA		3206			3.860	14.058		9.43
	ATOM	6322		TYR	3206		14.240	3.429	13.022		9.47
5	ATOM	6323	CB	TYR			14.310	1.895	13.023	1.00 39	
,			CG	TYR	3206		12.997	1.209	12.697		9.15
	ATOM	6324	CD1		3206		12.440	1.303	11.419	1.00 39	
	ATOM	6325	CE1	TYR	3206		11.226	0.707	11.113	1.00 39	
	MOTA	6326	CD2				12.298	0.486	13.670	1.00 39	
10	ATOM	6327	CE2		3206		11.065	-0.124	13.372		9.98
10	ATOM	6328	CZ	TYR	3206		10.536	-0.004	12.084		0.25
	ATOM	6329	ОН	TYR	3206		9.319	-0.576	11.753	1.00 40	
	ATOM	6330	C	TYR	3206		13.753	3.937	11.667	1.00 39	
	ATOM	6331	0	TYR	3206		12.625	4.406	11.547		69
15	ATOM	6332	И	LYS	3207		14.595	3.846	10.646		7.79
15	ATOM	6333	CA	LYS	3207		14.190	4.293	9.327		2.17
	ATOM	6334	CB	LYS	3207		14.907	5.593	8.953		3.85
	MOTA	6335	CG	LYS	3207		14.332	6.762	9.745		5.38
	ATOM	6336	CD	LYS	3207		14.807	8.122	9.287		3.03
20	MOTA	6337	CE	LYS	3207		13.873	9.190	9.850	1.00 48	
20	ATOM	6338	NZ	LYS	3207		14.296	10.584		.1.00 50	
	ATOM	6339	C	LYS	3207		14.383	3.229		- 1.00 42	
	ATOM	6340	0	LYS	3207		15.420	2.576	8.196	1:00 42	41
	MOTA	6341	N	VAL	3208		13.347	3.044	7.462	1.00 42	
05 .	ATOM	6342	CA	VAL	3208		13.368	2.056	6.404	1.00 42	
25	ATOM	6343	CB	VAL	3208		12.111	1.171	6.467	1.00 41	86
	ATOM	6344	CG1		3208		12.039	0.270	5.251	1.00 42	
	MOTA	6345		VAL	. 3208		12.137	0.344	7.728	1.00 42	.06
	MOTA.	6346	С	VAL	3208		13.401	2.758	5.060	1.00.43	.13
~~	MOTA	6347	0	VAL	3208		12.434	3.403	4.682	1.00 43	. 20
30	MOTA	6348	N	ARG	3209		14.521	2.661	4.352	1:00 43	.70
	MOTA	6349	CA	ARG	3209		14.608	3.268	3.033	1.00 44	.54
	ATOM	6350	CB	ARG	320.9		15.973	3.905	2.791	1.00 46	.46
	ATOM	6351	CG		. 3209		16.218	4.320	1.332	1.00 49	.71
	MOTA	6352	CD	ARG	3209		15.176		0.763		. 07
35 ·	MOTA	6353	NE	ARG	3209		13.801	4.795	0.746	1.00 53	
	MOTA	6354	CZ	ARG	3209		12.835	5.238	-0.062	1.00 53	
	MOTA	6355	NH1		3209		13.087	6.206	-0.936	1.00 53	
	ATOM	6356	NH2		3209		11.612	4.728	0.018	1.00 52	.96
40		6357	C	ARG	3209		14.386	2.150	2.036	1.00 44	.29
40	MOTA	6358	0	ARG	3209		15.274	1.326	1.797	1.00 44	.72
	MOTA	6359	N	TYR	3210		13.195	2.120	1.452	1.00 43	.42
	. ATOM	6360	CA	TYR	3210		12.844	1.081	0.495		.95
	MOTA	6361	CB	TYR	3210		11.393	1.239	0.050	1.00 43	.74
4.5	ATOM	6362	CG	TYR	3210	•	10.431	1.048	1.177		.73
45	ATOM	6363	CD1		3210		10.254	2.042	2.134	1.00 45	. 66
	MOTA	6364	CE1		3210		9.468	1.827	3.254	1.00 47	
	MOTA	6365	CD2	TYR	3210		9.785	-0.171	1.359	1.00 45	. 97
	MOTA	6366	CE2	TYR	3210		8.995	-0.405	2.477	1.00 46	.88
	MOTA	6367	CZ	TYR	3210		8.846	0.595	3.423		.53
50	ATOM	6368	OH	TYR	3210		8.113	0.349	4.564	1.00 49	.31
	ATOM	6369	C	TYR	3210		13.716	1.041	-0.733	1.00 42	.28
	ATOM	6370	0	TYR	3210		13.968	-0.027	-1.286	1.00 42	.12
	ATOM	6371	N	ALA	3211		14.167	2.204	-1.173	1.00 41	.86
	ATOM	6372	CA	ALA	3211	•	14.992	2.267	-2.368	1.00 41	.16
55	ATOM	6373	CB	ALA	3211		15.335	3.706	-2.680	1.00 41	
	ATOM	6374	C	ALA	3211		16.260	1.448	-2.205	1.00 40	
	ATOM	6375	0	ALA	3211		16.771	0.885	-3.169	1.00 41	
	ATOM	6376	N	THR	3212		16.760	1.375	-0.977	1.00 40	
	ATOM	6377	CA.	THR	3212		17.986	0.637	-0.711	1.00 39	
60	ATOM	6378	CB	THR	3212		18.996	1.527	0.053	1.00 40	
	ATOM	6379	OG1	THR	3212		18.385	2.033	1.251	1.00 40	
	ATOM	6380	CG2		3212		19.437	2.696	-0.826	1.00 39	

	3 max-	500	_		2010					
	ATOM	6381	C	THR	3212		17.736	-0.640	0.080	1.00 38.77
	ATOM	6382	0	THR	3212		18.675	-1.279	0.552	1.00 38.32
	MOTA	6383	N	TRP	3213		16.467	-1.004	0.223	1.00 38.07
5	ATOM	6384	CA	TRP	3213		16.095	-2.208	0.955	1.00 37.69
3	ATOM	6385	СВ	TRP	3213		16.415	-3.445	0.113	1.00 38.71
	ATOM	6386	CG	TRP	3213		15.801	-3.410	-1.260	1.00 39.88
	MOTA	6387		2 · TRP	3213		14.547	-3.981	-1.644	1.00 39.78
	MOTA	6388	CE2	TRP	3213		14.338	-3.659	-3.004	1.00 39.97
	MOTA.	6389	CES	TRP	3213		13.576	-4.733	-0.968	1.00 39.38
10	ATOM	6390	CD3	TRP	3213		16.294	-2.780	-2.379	1:00 39.94
	ATOM	6391	NE1	TRP	3213		15.418	-2.926	-3.429	1.00 39.80
	ATOM	6392	CZZ		3213		13.195	-4.066	-3.701	1.00 40.13
	ATOM	6393	CZ3		3213		12.441	-5.137	-1.660	
	ATOM	6394		TRP	3213		12.260	-4.803	-3.014	
15	ATOM	6395	C	TRP	3213		16.840	-2.281		1.00 39.80
	ATOM	6396	ŏ	TRP	3213				2.282	1.00 37.23
	ATOM	6397		SER			17.426	-3.308	2.627	1.00 36.36
			N		3214		16.812	-1.186	3.030	1.00 36.58
	ATOM	6398	CA	SER	3214		17.522	-1.163	4.293	1.00 36.48
20	ATOM	6399	CB	SER	3214		18.835	-0.406	4.124	1.00 36.91
20	ATOM	6400	OG	SER	3214		18.589	0.858	3.540	1:00 38.53
	MOTA	6401	С	SER	3214		16.736	-0.587	5.454	1.00 35.52
į	MOTA	6402	0	SER	3214	•	15,722	0.096	. ,5:277	1.00 34.85
	MOTA	6403	N	ILE	3215		17.215	-0.913	6.647	1.00 34.36
	ATOM	64.04	CA	ILE	3215		16.636	-0.443	7.888	1.00 33.91
25	MOTA	6405	CB	ILE	3215		16.002	-1.599	8.670	1.00 33.92
	ATOM	6406	CG2		3215		17.015	-2.680	8.920	1.00 34.47
	ATOM	6407	CG1		3215		15.427	-1.077	9.979	1.00 34.07
	ATOM	6408	CD1		3215		14.706	-2.131		1.00 34.38
	ATOM	6409	c	ILE	3215		17.806	0.151	8.661	
30	ATOM	6410	ŏ	ILE	3215		18.872	-0.454		1.00 33.13
	ATOM	6411	N	ILE	3216		17.616		8.742	1.00 32.83
	ATOM	6412	CA	ILE				1.352	9.194	1.00 32.76
	ATOM	6413			3216		18.667	2.036	9.936	1.00 32.20
			CB	.lle	3216		18.963	3.429	9.342	1.00 32.44
35	MOTA	6414	CG2		3216		20.110	4.086	10.088	1.00 31.04
33	MOTA	6415	CG1		3216		19.286	3.308	7.857	1.00 33.28
	ATOM	6416	CD1		3216		19.352	4.649	7.157	1.00 33.75
	" ATOM	6417	C	ILE	3216	•	18.257	2.265	11.377	1.00 31.96
	MOTA	6418	0	ILE	3216		17.158	2.754	11.638	1.00 31.00
40	ATOM	6419	И	MSE	3217		19.138	1.903	12.306	1.00 31.79
40.	MOTA	6420	CA	MSE	3217		18.880	2.136	13.716	1.00 31.79
	ATOM	6421	CB	MSE	3217		18.840	0.820	14.508	1.00 31.42
	ATOM	6422	CG	MSE	3217		17.603	-0.064	14.255	1.00 31.42
	. ATOM	6423	SE	MSE	3217		17.504	-1.556	15.341	1.00 31.78
	MOTA	6424	CE	MSE	3217		18.604	-2.673	14.447	1.00 30.54
45	MOTA	6425	C	MSE	3217		20.021	3.022	14.207	1.00 32.32
	MOTA	6426	0	MSE	3217		21.197	2.661	14.114	1.00 32.43
	ATOM	6427	Ŋ	ASP	3218		19.664	4.194	14.713	1.00 32.71
	ATOM	6428	CA	ASP	3218		20.628	5.147	15.229	
	ATOM	6429	CB	ASP	3218		20.022			1.00 33.09
50	MOTA	6430						6.544	15.123	1.00 35.67
-	ATOM	6431	CG	ASP	3218		21.063	7.625	15.018	1.00 38.30
	ATOM	6432		ASP	3218		20.843	8.702	15.618	1.00 39.16
				ASP	3218		22.089	7.401	14.327	1.00 40.02
	ATOM	6433	C	ASP	3218		20.927	4.813	16.696	1.00 32.45
55	ATOM	6434	0	ASP	3218		20.043	4.380	17.417	1.00 32.49
55	ATOM	6435	N	SER	3219		22.174	5.014	17.125	1.00 32.52
	ATOM .	6436	CA	SER	3219		22.611	4.753	18.505	1.00 31.30
•	ATOM	6437	CB	SER	3219		22.279	5.934	19.416	1.00 30.55
	ATOM	6438	OG	SER	3219		22.987	7.080	19.009	1.00 31.34
	MOTA	6439	С	SER	3219		22.046	3.496	19.143	1.00 30.80
60	ATOM	6440	0	SER	3219		21.242	3.578	20.073	1.00 31.63
	ATOM	6441	N	VAL	3220		22.473	2.335	18.663	1.00 29.85
	ATOM	6442	CA	VAL	3220		21.990	1.084	19.223	
•										1.00 29.07

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ATOM
              6443
                     CB
                         VAL
                               3220
                                          22.536
                                                   -0.142
                                                            18.423
                                                                     1.00 29.06
      ATOM
              6444
                     CG1 VAL
                               3220
                                          22.155
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                                                            16.960
                                                                     1.00 28.03
      ATOM
              6445
                     CG2 VAL
                               3220
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              6446
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                         VAL
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      ATOM
              6447
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                         VAL
                               3220
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      ATOM
              6451
                     CG1
                         VAL
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      ATOM
                     CG2 VAL
              6452
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                         PRO
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                         PRO
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                    СВ
                         PRO
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              6459
      ATOM
                    CG
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      ATOM
              6460
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                         PRO
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                         PRO
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                                                   -3.173
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                         SER
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                         SER
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                              3223
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      ATOM
              6465
                    OG
                         SER
      MOTA
              6466
                         SER
                    С
                              3223
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25
      ATOM
              6467
                         SER
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              6797
                    N
                         THR
                               3266
                                                             61.497
                                                                      1.00 39.76
     MOTA
              6798
                    CA
                         THR
                               3266
                                          44.372 -13.993
                                                             62.725
                                                                      1.00 40.06
                                          43.57.2 -13.479
43.477 -12.047
     MOTA
              6799
                               3266
                    CB
                         THR
                                                             63.938
                                                                      1.00 39.58
     ATOM
              6800
                    OG1 THR
                               3266
                                                             63.868
                                                                      1.00
                                                                           40.05
     MOTA
              6801
                    CG2 THR
                               3266
                                          44.240 -13.892
                                                             65.244
                                                                      1.00 38.53
50 .
     MOTA
              6802
                         THR
                               3266
                                                             62.790
                    C
                                        44.503 -15.509
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                                          43.504 -16.211
45.723 -16.025
     MOTA
              6803
                    0
                         THR
                               3266
                                                             62.879
                                                                      1.00 40.94
                               3267
                                                             62.710
     MOTA
              6804
                         VAL
                    N
                                                                      1.00 40.91
     MOTA
              6805
                    CA
                         VAL
                               3267
                                          45.894 -17.467
                                                             62.776
                                                                      1.00 41.66
                                          46.152 -18.085
45.047 -17.681
     MOTA
              6806
                                                             61.390
                   · CB
                         VAL
                               3267
                                                                      1.00 41.15
55
     MOTA
             6807
                         VAL
                               3267
                    CG1
                                                             60.442
                                                                      1.00 41.40
                                                             60.867
     MOTA
             6808
                    CG2
                         VAL
                               3267
                                          47.524 -17.662
                                                                      1.00 41.44
                                          47.015 -17.896
     MOTA
             6809
                         VAL
                               3267
                                                             63.706
                    C
                                                                      1.00 42.68
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     MOTA
             6810
                         VAL
                               3267
                                          47.886 -17.100
                                                             64.075
     MOTA
                               3268
             6811
                         ALA
                                          46.975 -19.170
                    N
                                                             64.086
                                                                      1.00 43.67
60
     MOTA
             6812
                    CA
                         ALA
                               3268
                                          47.971 -19.740
                                                             64.977
                                                                      1.00 44.57
                                          47.428 -21.008
     MOTA
                         ALA
                                                            65.622
             6813
                    CB
                               3268
                                                                      1.00 43.49
                                          49.243 -20.043
                                                                      1.00 45.06
     ATOM
             6814
                    C
                         ALA
                               3268
                                                             64.193
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ATOM 6816 N LEU 3269 50.375 -19.950 64.872 1.00 ATOM 6818 CB LEU 3269 51.653 -20.216 64.233 1.00 ATOM 6818 CB LEU 3269 52.769 -20.180 65.281 1.00 ATOM 6820 CD1 LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6821 CD2 LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6821 CD2 LEU 3269 54.755 -20.560 63.809 1.00 ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6824 N GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6825 CA GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.994 -22.523 64.093 1.00 ATOM 6827 O GLY 3270 50.991 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.861 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.861 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.644 -21.608 60.616 1.00 ATOM 6833 O SER 3271 47.644 -21.608 66.616 1.00 ATOM 6834 N ASN 3272 48.080 -22.274 58.653 1.00 ATOM 6835 CB ASN 3272 48.080 -22.286 55.601 1.00 ATOM 6836 CB SER 3271 49.000 -22.274 58.653 1.00 ATOM 6837 CG ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6838 N SER 3271 50.043 -21.747 58.252 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 N SER 3271 50.043 -21.747 58.252 1.00 ATOM 6836 CB ASN 3272 49.658 -22.644 57.840 1.00 ATOM 6837 CG ASN 3272 49.658 -22.644 57.840 1.00 ATOM 6838 N SER 3271 50.043 -21.747 58.252 1.00 ATOM 6838 N SER 3271 50.043 -21.747 58.252 1.00 ATOM 6838 N SER 3271 50.043 -21.747 58.252 1.00 ATOM 6840 C ASN 3272 49.658 -22.644 57.840 1.00 ATOM 6840 C ASN 3272 49.658 -22.644 57.840 1.00 ATOM 6840 C ASN 3272 49.658 -22.644 57.840 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C ASN 3272 49.655 -18.071 56.093 1.00 ATOM 6840 C	48.33 48.31 47.95 48.23 48.46 48.73 48.85 48.59 48.74 48.72 48.30 48.90 48.85
ATOM 6817 CA LEU 3269 51.653 -20.216 64.233 1.00 ATOM 6819 CG LEU 3269 52.769 -20.180 65.281 1.00 ATOM 6820 CD1 LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6821 CD2 LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6822 C LEU 3269 55.011 -19.389 66.030 1.00 ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6825 CA GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6826 C GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 47.042 -21.686 61.983 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6837 CG ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6838 OD1 ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 CD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6837 CG ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6838 CD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6837 CG ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6836 CD3 ASN 3272 49.655 -24.606 54.116 1.00 ATOM 6837 CG ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6838 CD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.788 1.00 ATOM 6841 O ASN 3272 49.655 -16.70 55.390 1.00 ATOM 6848 CQ VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6848 CD3 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6848 CD3 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6848 CD3 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6855 CD GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CD GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6858 CD GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6856 CD GLU 3274 44.998 -18.056 51.745 1.00 ATOM 6856 CD GLU 3274 44.1569 -20.769 5	47.35 47.80 48.41 48.33 48.31 48.23 48.23 48.46 48.73 48.82 48.59 48.74 48.70 48.80 48.70 48.80 48
ATOM 6817 CA LEU 3269 51.653 -20.216 64.233 1.00 ATOM 6819 CG LEU 3269 52.769 -20.180 65.281 1.00 ATOM 6820 CD1 LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6821 CD2 LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6822 C LEU 3269 55.011 -19.389 66.030 1.00 ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6825 CA GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6826 C GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 47.042 -21.686 61.983 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6837 CG ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6838 OD1 ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 CD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6837 CG ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6838 CD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6837 CG ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6836 CD3 ASN 3272 49.655 -24.606 54.116 1.00 ATOM 6837 CG ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6838 CD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.788 1.00 ATOM 6841 O ASN 3272 49.655 -16.70 55.390 1.00 ATOM 6848 CQ VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6848 CD3 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6848 CD3 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6848 CD3 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6855 CD GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CD GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6858 CD GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6856 CD GLU 3274 44.998 -18.056 51.745 1.00 ATOM 6856 CD GLU 3274 44.1569 -20.769 5	47.35 47.80 48.41 48.33 48.31 48.23 48.23 48.46 48.73 48.82 48.59 48.74 48.70 48.80 48.70 48.80 48
ATOM 6818 CB LEU 3269 52,769 -20,180 65,281 1.00 ATOM 6820 CD1 LEU 3269 54,112 -19,616 64,818 1.00 ATOM 6821 CD2 LEU 3269 55,011 -19,389 66,030 1.00 ATOM 6822 C LEU 3269 51,596 -21,587 63,564 1.00 ATOM 6823 O LEU 3269 50,994 -22,523 64,093 1.00 ATOM 6825 CA GLY 3270 52,206 -21,699 62,390 1.00 ATOM 6826 C GLY 3270 50,971 -23,257 60,861 1.00 ATOM 6827 O GLY 3270 50,896 -24,291 60,189 1.00 ATOM 6827 O GLY 3271 49,992 -22,357 60,904 1.00 ATOM 6830	47.80 48.41 48.33 48.31 47.95 48.46 48.23 48.46 48.73 48.59 48.74 48.70 48.70 48.70 48.80 48.70 48.80 48
5 ATOM 6819 CG LEU 3269 54.112 -19.616 64.818 1.00 ATOM 6821 CD2 LEU 3269 55.011 -19.389 66.030 1.00 ATOM 6821 CD2 LEU 3269 54.755 -20.560 63.809 1.00 ATOM 6822 C LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6824 N GLY 3270 52.206 -21.587 63.564 1.00 ATOM 6825 CA GLY 3270 50.991 -22.257 60.0861 1.00 ATOM 6826 C GLY 3270 50.896 -24.291 60.189 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM	48.41 48.33 48.31 47.95 48.23 48.46 48.73 48.74 48.72 48.74 48.72 48.89 48.85 48.74 48.90 48.85 48
ATOM 6820 CD1 LEU 3269 55.011 -19.389 66.030 1.00 ATOM 6821 CD2 LEU 3269 54.755 -20.560 63.809 1.00 ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6824 N GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6825 CA GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.991 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.644 -21.608 60.616 1.00 ATOM 6833 O SER 3271 49.900 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6835 CA ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6836 CB ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6839 ND2 ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.655 -24.606 54.116 1.00 ATOM 6842 N VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6844 CB VAL 3273 47.890 -19.314 55.148 1.00 ATOM 6845 CG1 VAL 3273 47.890 -19.314 55.148 1.00 ATOM 6846 CG2 VAL 3273 47.890 -19.315 55.390 1.00 ATOM 6847 C VAL 3273 47.890 -19.315 55.390 1.00 ATOM 6848 O VAL 3273 47.890 -19.315 55.190 1.00 ATOM 6848 O VAL 3273 47.890 -19.317 55.929 1.00 ATOM 6848 O VAL 3273 47.890 -19.317 55.929 1.00 ATOM 6848 O VAL 3273 47.890 -19.315 55.1850 1.00 ATOM 6848 O VAL 3273 47.890 -19.515 55.0929 1.00 ATOM 6848 O VAL 3273 47.890 -19.515 55.093 1.00 ATOM 6848 O VAL 3273 47.890 -19.515 55.093 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6850 CA GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6850 CC GLU 3274 44.998 -18.056 51.745 1.00 ATOM 6855 CC GLU 3274 44.999 -16.768 51.745 1.00	48.33 48.31 47.95 48.23 48.46 48.73 48.82 48.59 48.74 48.72 48.30 48.85 48.72 48.85 48.85 48.85 48.85 48.85
ATOM 6821 CD2 LEU 3269 54.755 -20.560 63.809 1.00 ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6824 N GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6825 CA GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 49.900 -22.274 58.653 1.00 ATOM 6834 N ASN 3272 48.020 -22.274 58.653 1.00 ATOM 6835 CA ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6836 CB ASN 3272 48.000 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.0648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.018 50.00 ATOM 6840 C	48.31 47.95 48.23 48.46 48.73 48.82 48.59 48.74 48.30 48.30 48.30 48.85 48.90 48.65
ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6823 O LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6824 N GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.961 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.961 1.00 ATOM 6827 O GLY 3270 50.971 -23.257 60.961 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6834 N ASN 3272 48.080 -22.3644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.953 -24.469 55.374 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.655 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 49.655 -24.606 54.116 1.00 ATOM 6842 N VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6843 CA VAL 3273 47.299 -20.337 55.390 1.00 ATOM 6844 CB VAL 3273 46.505 -18.071 55.093 1.00 ATOM 6846 CG2 VAL 3273 47.782 -19.251 56.929 1.00 ATOM 6847 C VAL 3273 47.782 -19.251 56.929 1.00 ATOM 6848 O VAL 3273 47.589 -19.251 56.929 1.00 ATOM 6848 O VAL 3273 47.589 -19.251 56.929 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6848 O VAL 3273 47.592 -18.984 53.217 1.00 ATOM 6848 O VAL 3273 47.592 -18.984 53.217 1.00 ATOM 6848 O VAL 3273 47.592 -18.984 53.217 1.00 ATOM 6848 O VAL 3273 47.592 -18.984 53.217 1.00 ATOM 6848 O VAL 3273 47.592 -18.924 53.011 1.00 ATOM 6840 CG VAL 3273 47.592 -18.924 53.011 1.00 ATOM 6840 CG VAL 3273 47.592 -18.924 53.011 1.00 ATOM 6840 CG VAL 3273 47.592 -18.924 53.011 1.00 ATOM 6850 CG GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6850 CG GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6850 CG GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6850 CC GLU 3274 44.999 -16.768 51.745 1.00	47.95 48.23 48.46 48.73 48.82 48.59 48.74 48.72 48.85 48.90 48.90 48.65
ATOM 6822 C LEU 3269 51.596 -21.587 63.564 1.00 ATOM 6824 N GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6825 CA GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.904 1.00 ATOM 6827 C GLY 3270 50.971 -23.257 60.904 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 49.000 -22.274 58.653 1.00 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.053 -24.4606 54.116 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.953 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 49.953 -24.606 54.116 1.00 ATOM 6840 C ASN 3272 49.953 -24.606 54.116 1.00 ATOM 6840 C ASN 3272 49.953 -55.374 1.00 ATOM 6840 C ASN 3272 49.953 -55.374 1.00 ATOM 6840 C ASN 3272 49.655 -56.718 1.00 ATOM 6840 C ASN 3272 49.655 -56.718 1.00 ATOM 6840 C ASN 3272 49.953 -54.695 55.601 1.00 ATOM 6840 C ASN 3272 49.953 -54.695 55.601 1.00 ATOM 6840 C ASN 3272 49.953 -54.695 55.601 1.00 ATOM 6840 C ASN 3272 49.953 -54.695 55.601 1.00 ATOM 6840 C ASN 3272 49.953 -54.695 55.601 1.00 ATOM 6840 C ASN 3272 49.953 -54.695 55.601 1.00 ATOM 6840 C ASN 3272 49.953 -55.374 55.390 1.00 ATOM 6840 C ASN 3272 45.898 -21.457 56.748 1.00 ATOM 6840 C ASN 3272 45.898 -21.457 55.390 1.00 ATOM 6840 C ASN 3272 45.898 -21.457 55.148 1.00 ATOM 6840 C ASN 3272 45.898 -21.457 55.992 1.00 ATOM 6840 C ASN 3273 47.802 -19.314 55.148 1.00 ATOM 6840 C ASN 3272 45.898 -21.457 55.992 1.00 ATOM 6840 C ASN 3273 47.802 -18.924 53.011 1.00 ATOM 6840 C Q VAL 3273 47.802 -18.924 53.011 1.00 ATOM 6850 C G GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6850 CA GLU 3274 44.998 -18.056 51.850 1.00 ATOM 6850 C G GLU 3274 44.999 -16.768 51.745 1.00 ATOM 6850 C G GLU 3274 44.999 -16.768 51	48.23 48.46 48.73 48.82 48.59 48.74 48.72 48.30 48.85 48.90 48.85 48.90 48.65
10 ATOM 6823 O LEU 3269 50.994 -22.523 64.093 1.00 ATOM 6824 N GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6825 CA GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 47.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6834 N ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6830 ND2 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.645 -24.666 54.116 1.00 ATOM 6841 O ASN 3272 49.645 -24.666 54.116 1.00 ATOM 6840 C ASN 3272 49.645 -25.012 56.318 1.00 ATOM 6841 CB VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6850 CA GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CC GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CC GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6856 C GLU 3274 43.397 -21.900 50.214 1.00	48.23 48.46 48.73 48.82 48.59 48.74 48.72 48.30 48.85 48.90 48.85 48.90 48.65
10 ATOM 6824 N GLY 3270 52.206 -21.699 62.390 1.00 ATOM 6825 CA GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 49.000 -22.274 58.653 1.00 ATOM 6835 CA ASN 3272 48.080 -22.366 56.412 1.00 ATOM 6835 CA ASN 3272 48.080 -22.366 55.601 1.00 ATOM 6836 CB ASN 3272 49.005 -22.644 57.840 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25:012 56.318 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25:012 56.318 1.00 ATOM 6840 C ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 49.465 -24.457 56.748 1.00 ATOM 6840 C ASN 3272 49.465 -24.457 56.748 1.00 ATOM 6841 CASN 3273 46.290 -19.314 55.148 1.00 ATOM 6840 CASN 3273 46.290 -19.314 55.148 1.00 ATOM 6846 CG2 VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6846 CG2 VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6847 C VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6846 CG2 VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6847 C VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6846 CG2 VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6847 C VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6848 O VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6848 O VAL 3273 46.505 -16.770 55.280 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CB GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CB GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CB GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CB GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CB GLU 3274 44.989 -18.056 51.850 1.00 ATOM 6855 CB GLU 3274 44.989 -18.056 51.850 1.00	48.46 48.73 48.82 48.59 48.74 48.72 48.30 48.90 48.90 48.90 48.65
ATOM 6825 CA GLY 3270 52.214 -22.966 61.683 1.00 ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.896 -24.291 60.189 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 15 ATOM 6829 CA SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6840 C ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 45.898 -21.457 56.748 1.00 ATOM 6841 O ASN 3272 45.898 -21.457 56.748 1.00 ATOM 6843 CA VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6844 CB VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6846 CG2 VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6847 C VAL 3273 46.595 -18.514 53.217 1.00 ATOM 6848 O VAL 3273 46.565 -16.770 55.280 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6854 OE1 GLU 3274 44.988 -18.056 50.363 1.00 ATOM 6854 OE1 GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6854 OE1 GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6854 OE1 GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6854 OE1 GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6854 OE1 GLU 3274 44.988 -19.056 51.325 1.00 ATOM 6855 CC GLU 3274 44.989 -19.766 51.00 ATOM 6854 OE1 GLU 3274 44.189 -16.768 51.745 1.00	48.73 48.82 48.59 48.74 48.70 48.70 48.90 48.85 48.85 48.85 48.65
ATOM 6826 C GLY 3270 50.971 -23.257 60.861 1.00 ATOM 6827 O GLY 3270 50.896 -24.291 60.189 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6829 CA SER 3271 47.644 -21.608 60.616 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.766 61.983 1.00 ATOM 6832 C SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 20 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6836 CB ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6839 ND2 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.648 -25.012 56.748 1.00 ATOM 6842 N VAL 3273 46.992 -21.353 56.185 1.00 ATOM 6843 CA VAL 3273 46.992 -21.353 56.185 1.00 ATOM 6844 CB VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6846 CG2 VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6853 CD GLU 3274 44.988 -18.056 50.926 1.00 ATOM 6854 OE1 GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6855 CD GLU 3274 44.988 -18.056 51.955 1.00 ATOM 6854 OE1 GLU 3274 44.988 -19.056 51.955 1.00 ATOM 6855 CD GLU 3274 44.189 -16.768 51.745 1.00	48.82 48.59 48.74 48.72 48.30 48.85 48.85 48.90 48.65
ATOM 6827 O GLY 3270 50.896 -24.291 60.189 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 47.312 -21.786 61.983 1.00 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6836 CB ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6837 CG ASN 3272 49.080 -22.386 55.601 1.00 ATOM 6838 ODI ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6839 ND2 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6842 N VAL 3273 46.992 -21.353 56.185 1.00 ATOM 6843 CA VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 55.280 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6849 N GLU 3273 46.505 -18.071 55.280 1.00 ATOM 6847 C VAL 3273 46.505 -18.888 53.696 1.00 ATOM 6848 O VAL 3273 46.505 -18.888 53.696 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CD GLU 3274 44.699 -19.780 51.325 1.00 ATOM 6855 CD GLU 3274 44.699 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 44.699 -10.768 51.745 1.00 ATOM 6855 OE2 GLU 3274 44.689 -10.768 51.745 1.00	48.59 48.74 48.72 48.30 48.90 48.85 48.72 48.90 48.65
ATOM 6827 O GLY 3270 50.896 -24.291 60.189 1.00 ATOM 6828 N SER 3271 49.992 -22.357 60.904 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.644 -21.608 60.616 1.00 ATOM 6832 C SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 47.312 -21.786 61.983 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6842 N VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6843 CA VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6845 CG1 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 55.280 1.00 ATOM 6847 C VAL 3273 46.505 -18.888 53.696 1.00 ATOM 6848 O VAL 3273 46.505 -18.888 53.696 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CD GLU 3274 44.421 -19.156 50.926 1.00 ATOM 6855 CD GLU 3274 44.421 -19.156 50.926 1.00 ATOM 6855 CD GLU 3274 44.421 -19.156 50.926 1.00 ATOM 6855 CD GLU 3274 44.421 -19.156 50.926 1.00 ATOM 6855 CD GLU 3274 44.698 -18.056 51.325 1.00 ATOM 6855 CD GLU 3274 44.689 -18.056 51.325 1.00 ATOM 6855 CD GLU 3274 44.699 -16.768 51.745 1.00 ATOM 6855 CD GLU 3274 44.699 -16.768 51.745 1.00	48.74 48.72 48.30 48.90 48.85 48.72 48.90 48.65
ATOM	48.74 48.72 48.30 48.90 48.85 48.72 48.90 48.65
15 ATOM 6829 CA SER 3271 48.763 -22.552 60.135 1.00 ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 20 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 46.992 -21.353 56.185 1.00 ATOM 6842 N VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6843 CA VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6844 CB VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.929 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.929 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.929 1.00 ATOM 6849 N GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6850 CG GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.325 1.00 ATOM 6853 CD GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6855 OCE GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 OCE GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 OCE GLU 3274 44.6653 -20.897 50.363 1.00 ATOM 6855 OCE GLU 3274 44.6653 -20.769 49.756 1.00 ATOM 6855 OCE GLU 3274 44.189 -16.768 51.745 1.00	48.72 48.30 48.90 48.85 48.72 48.90 48.65
ATOM 6830 CB SER 3271 47.644 -21.608 60.616 1.00 ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6839 ND2 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 46.992 -21.353 56.185 1.00 ATOM 6842 N VAL 3273 46.992 -21.353 56.185 1.00 ATOM 6843 CA VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6844 CB VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6849 N GLU 3274 46.505 -18.071 55.280 1.00 ATOM 6849 N GLU 3273 46.505 -18.071 56.093 1.00 ATOM 6849 N GLU 3273 46.505 -18.071 56.093 1.00 ATOM 6849 N GLU 3273 46.505 -18.071 56.093 1.00 ATOM 6849 N GLU 3274 46.505 -18.514 53.217 1.00 ATOM 6850 CA GLU 3274 45.095 -18.514 53.217 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CG GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CG GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6855 CG GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6855 CG GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 CC GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 CC GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 CC GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 CC GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 CC GLU 3274 44.189 -16.768 51.745 1.00	48.30 48.90 48.85 48.72 48.90 48.65
ATOM 6831 OG SER 3271 47.312 -21.786 61.983 1.00 ATOM 6832 C SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 20 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 25 ATOM 6839 ND2 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6841 O ASN 3272 49.649 -22.353 56.185 1.00 ATOM 6842 N VAL 3273 46.992 -21.353 56.185 1.00 ATOM 6843 CA VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6844 CB VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6845 CG1 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6847 C VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 46.505 -18.071 56.929 1.00 ATOM 6849 N GLU 3274 46.565 -16.770 55.280 1.00 ATOM 6849 N GLU 3274 46.505 -18.924 53.011 1.00 ATOM 6849 N GLU 3274 45.095 -18.514 53.217 1.00 ATOM 6850 CA GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6850 CA GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6850 CB GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6850 CB GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6850 CB GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6850 CB GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 OE2 GLU 3274 41.899 -16.768 51.745 1.00	48.90 48.85 48.72 48.90 48.65
ATOM 6832 C SER 3271 49.000 -22.274 58.653 1.00 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 OD1 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6839 ND2 ASN 3272 49.648 -25.012 56.318 1.00 ATOM 6840 C ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 45.898 -21.457 56.748 1.00 ATOM 6842 N VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6843 CA VAL 3273 46.290 -19.314 55.148 1.00 ATOM 6844 CB VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6848 O VAL 3273 47.782 -18.251 56.929 1.00 ATOM 6848 O VAL 3273 46.565 -16.770 55.280 1.00 ATOM 6848 O VAL 3273 46.575 -18.888 53.696 1.00 ATOM 6848 O VAL 3273 47.782 -18.251 56.929 1.00 ATOM 6848 O VAL 3273 47.59 -18.888 53.696 1.00 ATOM 6848 O VAL 3273 47.30 -18.888 53.696 1.00 ATOM 6848 O VAL 3273 47.30 -18.888 53.696 1.00 ATOM 6848 O VAL 3273 47.30 -18.924 53.011 1.00 ATOM 6850 CA GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 CD GLU 3274 44.421 -19.156 50.926 1.00 ATOM 6856 C GLU 3274 42.653 -20.897 50.363 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 41.562 -20.769 49.756 1.00 ATOM 6855 OE2 GLU 3274 41.899 -16.768 51.745 1.00	48.85 48.72 48.90 48.65
20 ATOM 6833 O SER 3271 50.043 -21.747 58.252 1.00 20 ATOM 6834 N ASN 3272 48.020 -22.644 57.840 1.00 ATOM 6835 CA ASN 3272 48.080 -22.386 56.412 1.00 ATOM 6836 CB ASN 3272 47.800 -23.656 55.601 1.00 ATOM 6837 CG ASN 3272 49.053 -24.489 55.374 1.00 ATOM 6838 ODI ASN 3272 49.648 -25.012 56.318 1.00 25 ATOM 6839 ND2 ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6840 C ASN 3272 49.465 -24.606 54.116 1.00 ATOM 6841 O ASN 3272 45.898 -21.457 56.748 1.00 ATOM 6842 N VAL 3273 47.289 -20.337 55.390 1.00 ATOM 6843 CA VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6844 CB VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.093 1.00 ATOM 6846 CG2 VAL 3273 46.505 -18.071 56.929 1.00 ATOM 6847 C VAL 3273 46.565 -16.770 55.280 1.00 ATOM 6848 O VAL 3273 46.565 -16.770 55.280 1.00 ATOM 6848 O VAL 3273 46.505 -18.888 53.696 1.00 ATOM 6849 N GLU 3274 46.275 -18.888 53.696 1.00 ATOM 6850 CA GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6851 CB GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6852 CG GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6853 CD GLU 3274 44.988 -18.056 51.850 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 51.325 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.091 -19.780 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.397 -21.900 50.214 1.00 ATOM 6855 OE2 GLU 3274 43.397 -21.900 50.214 1.00	48.72 48.90 48.65
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ATOM 6861 CG PHE 3275 45.638 12.985 52.356 1.00	39.51
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ATOM 6867 C PHE 3275 43.534 -14.530 49.546 1.00	41.21
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ATOM 6872 CG MSE 3276 40.093 -15.885 48.719 1.00	41.77
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                                                           55.433
                                                                    1.00 80.16
      MOTA
              7062
                    0
                         LYS
                              3299
                                         59.013
                                                   0.594
                                                                    1.00 80.40
                                                           54.375
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	ATOM	7063	N	ILE	3300		59.213	2.538	55.501	1.00 79.98	
	ATOM	7064	CA	ILE			59.200			1.00 79.69	_
	ATOM	7065	CB	ILE	3300		58.723			1.00 79.63	
	ATOM	7066	CG2		3300		58.594	5.667		1.00 79.72	
5	ATOM	7067	CG1		3300		57.390	4.765		1.00 79.41	
	ATOM	7068	CD1		3300		56.253	4.116		1.00 79.32	
	ATOM	7069	С	ILE	3300		60.608	3.487	53.733	1.00 79.48	
	ATOM	7070	0	ILE	3300		61.594	3.289		1.00 79.39	
	ATOM	7071	N	GLY	3301		60.693	3.794	52.438	1.00 79.23	
10	ATOM	7072	CA	GLY	3301		61.984	3.901	51.776	1.00 78.75	
	ATOM	7073	· C	GLY	3301		62.391	5.314	51.396	1.00 78.43	
	MOTA	7074	0	GLY	3301		61.613	6.254	51.576	1.00 78.22	
	ATOM	7075	N	PRO	3302		63.617	5.495	50.869	1.00 78.33	
	ATOM	7076	CD	PRO	3302		64.630	4.432	50.715	1.00 78.24	
15	MOTA	7077	CA	PRO	3302		64.163	6.794	50.450	1.00 78.05	
	ATOM	7078	CB	PRO	3302		65.496	6.409	49.816	1.00 78.14	ĺ
	ATOM	7079	CG	PRO	3302		65.918	5.221	50.645	1.00 78.20	
	MOTA	.7080	C	PRO	3302		63.249	7.558	49.486		
	. ATOM	7081	0	PRO	3302		63.168	8.789	49.530	1.00 77.68	
20 .	ATOM	7082	N	ASP	3303		62.566	6.818	. 48.618	1.00 77.59	
	ATOM	7093	CA	ASP	3303		61.641	7.399	47.648	1.00 77.04	
	ATOM	7084	CB	ASP	3303	-	61.424	6.428	.46.488	1.00 77.64	
	MOTA	7085	CĠ	ASP	3303		61.114		46.960	1.00 78.74	
	ATOM	7086		ASP	3303		60.674	4,188	46.129	1.00 79.08	
25	ATOM	7087	OD2	ASP	3303		61.319	4.717	48.161	1.00 78.84	
	ATOM	7088	С	ASP	3303		60.294	7.717	48.302	1.00 76.37	
•	MOTA	7089	0	ASP	3303		59.315	8.013	47.615	1.00 76.40	
	MOTA	7090	N	ASN	3304		60.258	7.650	49.632	1.00 75.35	
<u>.</u>	MOTA	7091	CA	ASN	3304	•	59.055	7.923	50.419	1.00 74.01	
30	MOTA	7092	CB	ASN	3304	•	58.443	9.271	50.015	1.00 74.62	
	MOTA	7093	CG	asn	3304		57.289	9.686	50.919	1.00 75.31	
: .	MOTA	7094	OD1	ASN	3304 .		57.410	9.673.	52.150	1.00 74.78	
•	MO'LY	7095		ASN	3304		56.165	10.067	50.309	1.00 75.48	
25	ATOM	7096	Ç	ASN	3304		58.003	6.819	50.310	1.00 72.60	
35	ATOM	7097	0	ASN	3304		56:999	6.839	51.022	1.00 72.47	
	MOTA	7098	N	TEU	3305		58.231	5.858	49.419	1.00 70.90	
	ATOM ·	7099	CA	LEU	3305		57.298	4.749	49.253	1.00 69.05	
	ATOM	7100	СВ	LEU	3305		57.250	4.277	47.795	1.00 68.83	
40	ATOM	7101	CG	LEU	3305		56.744	5.246	46.721	1.00 68.36	
40	MOTA	7102	CD1		3305		55.696	6.181	47.310	1.00 67.98	
	ATOM ATOM	7103		LEU.			57.907	6.042	46.175	1.00 68.66	
	ATOM	7104 7105	C	LEU	3305		57.708	3.586	50.152	1.00 67.70	
	ATOM	7105	0	LEU	3305 3306		58.886	3.420	50.473	1.00 67.84	
45	ATOM	7107	ห CD	PRO	3306		56.731		50.575	1.00 65.95	
73	ATOM	7108	CA	PRO PRO	3306		55.285	2.974	50.366	1.00 65.41	
	ATOM	7109	CB	PRO	3306		56.972	1.608	51.445	1.00 64.27	
	ATOM	7110	CG	PRO	3306		55.570 54.701	1.274	51.955	1.00 64.68	
	ATOM	7111	C	PRO	3306		57.635	1.646	50.793	1.00 64.90	
50	ATOM	7112	ŏ	PRO	3306		57.341	0.415 0.125	50.747 49.585	1.00 62.31	
•	ATOM	7113		TYR	3307		58.528			1.00 62.30	
	ATOM	7114		TYR	3307	•	59.205	-0.273 -1.436	51.457	1.00 59.98	
	ATOM	7115		TYR	3307		60.361	-1.900	50.887	1.00 57.51	
	ATOM	7116		TYR	3307		61.474	-0.884	51.772	1.00 59.68	
55	ATOM	7117	CD1		3307		61.439	0.071	51.923 52.942	1.00 62.15	
	ATOM	7118	CE1		3307		62.465	1.006	52.942	1.00 63.18	
	ATOM	7119	CD2	ጥሃው	3307		62.566	-0.877		1.00 63.93	
	ATOM	7120	CE2	ጥሃ₽	3307		63.598	0.059	51.048 51.186	1.00 62.88	
	ATOM	71:21		TYR	3307		63.539	0.059	52.212	1.00 63.66	
60	ATOM.	7122		TYR	3307		64.549	1.920		1.00 64.25	
	ATOM	7123		TYR	3307		58.219	-2.575	52.365 .50.719	1.00 64.71 1.00 54.35	
	ATOM	7124		TYR	3307		57.352	-2.788	51.558	1 00 53 01	
			-		555,		37.332	2.700	21.330	1.00 53.91	

ATOM 7128 CG1 VAL 3308 55.379 5.379 5.379 48.388 1.00 45.81 ATOM 7130 CC2 VAL 3308 56.999 -3.211 47.204 1.00 45.81 ATOM 7131 0 VAL 3308 58.200 -3.515 48.171 1.00 46.58 ATOM 7132 N GLN 3309 57.627 -5.415 48.141 1.00 46.28 ATOM 7133 CG CAIN 3309 57.627 -5.415 48.141 1.00 46.50 48.10 ATOM 7134 CB GLN 3309 57.627 -7.962 48.249 1.00 44.02 ATOM 7135 CG GLN 3309 58.6601 -8.922 49.366 1.00 45.74 ATOM 7136 CD GLN 3309 58.6601 -8.922 49.366 1.00 45.74 ATOM 7137 OEL GLN 3309 58.6601 -8.922 49.566 1.00 47.62 ATOM 7138 NE2 GLN 3309 59.562 -11.155 50.11 1.00 49.24 ATOM 7139 CD GLN 3309 59.562 -11.255 50.11 1.00 49.24 ATOM 7130 CD GLN 3309 59.562 -11.255 50.11 1.00 49.24 ATOM 7130 CD GLN 3309 59.563 -10.888 51.184 1.00 50.266 ATOM 7134 CB GLN 3309 59.963 -10.888 51.184 1.00 50.266 ATOM 7134 CB GLN 3309 59.963 -10.888 51.184 1.00 50.266 ATOM 7140 CG GLN 3309 59.963 -10.888 51.184 1.00 49.10 ATOM 7141 CG GLN 3309 59.963 -10.888 51.184 1.00 42.94 ATOM 7142 CB LEE 3310 57.528 8.875 47.769 1.00 42.99 ATOM 7144 CG2 ILE 3310 57.528 8.874 46.055 1.00 41.35 ATOM 7145 CG1 ILE 3310 57.627 -7.753 43.450 1.00 41.19 ATOM 7146 CG1 ILE 3310 57.627 -7.753 43.450 1.00 41.19 ATOM 7146 CG1 ILE 3310 57.627 -7.753 43.450 1.00 41.19 ATOM 7146 CG1 ILE 3310 57.627 -7.753 43.450 1.00 40.25 ATOM 7146 CG1 ILE 3310 57.627 -7.753 43.450 1.00 40.25 ATOM 7146 CG1 ILE 3310 57.627 -7.753 43.450 1.00 40.25 ATOM 7146 CG1 ILE 3310 57.627 -7.753 43.450 1.00 40.25 ATOM 7150 CA LEU 3311 55.095 -12.667 46.108 1.00 39.96 ATOM 7150 CA LEU 3311 55.095 -12.667 46.108 1.00 39.94 ATOM 7150 CA LEU 3311 55.995 -12.667 46.108 1.00 39.94 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.94 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.94 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.94 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.94 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.94 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.95 ATOM 7150 CA LEU 3311 59.667 -7.7720 47.288 1.00 39.95 ATOM 7150 CA LEU 3311 59.		ATOM ATOM ATOM	7125 7126 7127	N CA CB	VAL VAL VAL	3308 3308 3308		57.474 -	-3.317 -4.418	49.632 49.335	1.00	50.61 47.32
ATOM 7130 C VAL 3308 58.210 -5.585 48.711 1.00 46.29 ATOM 7131 O VAL 3308 59.282 -5.415 48.142 1.00 46.29 ATOM 7132 N GLN 3309 57.627 -6.771 48.816 1.00 45.01 ATOM 7134 CB GLN 3309 58.621 -7.962 48.249 1.00 44.02 ATOM 7135 CC GLN 3309 58.621 -1.922 49.366 1.00 45.74 ATOM 7136 CD GLN 3309 59.662 -11.35 50.011 1.00 49.24 ATOM 7137 OEL GLN 3309 59.662 -11.35 50.011 1.00 49.24 ATOM 7138 NE2 GLN 3309 59.9662 -11.35 50.011 1.00 49.24 ATOM 7139 C GLN 3309 59.9662 -12.355 49.587 1.00 49.10 ATOM 7140 O GLN 3309 59.966 -10.888 51.184 1.00 50.266 ATOM 7141 N ILE 3310 55.058 -8.75 47.769 1.00 42.99 ATOM 7141 N ILE 3310 55.058 -8.75 47.769 1.00 43.03 ATOM 7142 CJ ILE 3310 55.058 -8.749 46.055 1.00 41.35 ATOM 7145 CGI ILE 3310 55.058 -9.166 43.650 1.00 41.19 ATOM 7146 CGI ILE 3310 55.925 -9.424 42.696 1.00 41.19 ATOM 7147 C ILE 3310 55.925 -9.424 42.696 1.00 41.19 ATOM 7148 O ILE 3310 55.458 -1.26 43.450 1.00 40.25 ATOM 7149 N LEU 3311 55.925 -9.424 42.696 1.00 40.25 ATOM 7149 N LEU 3311 55.925 -9.424 42.966 1.00 40.25 ATOM 7149 N LEU 3311 55.095 -12.667 46.108 1.00 39.96 ATOM 7150 CA LEU 3311 55.095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55.095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55.925 -9.424 42.966 1.00 39.95 ATOM 7150 CA LEU 3311 55.925 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55.925 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55.925 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55.925 -12.667 46.108 1.00 39.94 ATOM 7156 C LEU 3311 55.925 -12.255 42.943 1.00 39.94 ATOM 7156 C R LEU 3311 55.925 -12.255 42.943 1.00 39.94 ATOM 7156 C R LEU 3312 55.925 -12.502 41.852 1.00 39.94 ATOM 7156 C R LEU 3312 55.925 -12.502 41.852 1.00 39.95 ATOM 7160 CG LYS 3312 53.266 -17.752 42.942 1.00 39.91 ATOM 7157 C R LEU 3313 55.946 -12.251 49.494 1.00 39.93 ATOM 7156 C R LEU 3313 55.946 -12.251 49.940 1.00 39.95 ATOM 7157 C R LEU 3313 55.966 -11.921 39.996 1.00 39.95 ATOM 7160 CG LYS 3312 52.926 -11.921 39.996 1.00 39.95 ATOM 7176 C R LEU 3313 53.066 -10.200 40.196 1.00 40.95 ATOM 7177 C R ALA 3313 53.066 -	5	MOTA	7128	CG	L VAL	3308		55.379 -				45.81
ATOM 7131 O VAL 3308												
ATOM 7132 N GEN 3309 57.627 -6.771 48.816 1.00 44.02 ATOM 7133 CA GEN 3309 58.225 -7.962 48.249 1.00 44.02 ATOM 7135 CG GEN 3309 58.601 -8.932 49.366 1.00 45.74 ATOM 7136 CD GEN 3309 59.594 -10.024 48.969 1.00 47.62 ATOM 7137 OEI GEN 3309 59.963 -10.888 51.184 1.00 49.24 ATOM 7138 NE2 GEN 3309 59.963 -10.888 51.184 1.00 49.24 ATOM 7130 C GEN 3309 59.963 -10.888 51.184 1.00 49.10 ATOM 7140 O GEN 3309 59.376 -12.365 49.587 1.00 49.10 ATOM 7141 N LEE 3310 55.528 -8.749 46.055 1.00 41.39 ATOM 7141 N LEE 3310 55.528 -8.749 46.055 1.00 41.39 ATOM 7142 CA LLE 3310 55.529 -9.338 45.097 1.00 40.25 ATOM 7145 CGI LLE 3310 55.925 -9.424 42.696 1.00 41.19 ATOM 7146 CDI LLE 3310 55.6600 -6.672 43.306 1.00 41.79 ATOM 7147 C LLE 3310 55.6400 -6.672 43.306 1.00 41.79 ATOM 7148 O LLE 3310 55.495 -9.424 42.696 1.00 40.25 ATOM 7149 N LEU 3311 55.304 -11.266 45.312 1.00 39.96 ATOM 7155 CA LEU 3311 55.095 -12.667 46.108 1.00 39.93 ATOM 7151 CB LEU 3311 55.095 -12.667 46.108 1.00 39.93 ATOM 7155 CA LEU 3311 55.406 -12.251 49.630 1.00 39.14 ATOM 7156 O LEU 3311 55.406 -12.251 49.630 1.00 39.14 ATOM 7156 O LEU 3311 55.406 -12.251 49.630 1.00 39.14 ATOM 7156 CB LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.14 ATOM 7156 O LEU 3311 55.595 -12.667 46.108 1.00 39.30 ATOM 7157 N LYS 3312 53.846 -12.251 49.630 1.00 39.14 ATOM 7157 C B LSU 3311 55.595 -12.667 46.108 1.00 39.30 ATOM 7157 O ALS 3312 53.266 -11.3525 42.943 1.00 39.30 ATOM 7157 O ALS 3312 55.946 -11.267 38.305 1.00 39.20 ATOM 7157 O ALS 3312 55.946 -11.267 38.305 1.00 39.30 ATOM 7157 O ALS 3312 55.946 -11.267 38.305 1.00 39.30 ATOM 7157 O ALS 3312 55.946 -11.267 38.305 1.00 39.30 ATOM 7157 O ALS 3313 55.466 -12.677 38.305 1.00 39.30 ATOM 7158 C A LYS 3312 55.946 -11.267		ATOM	7131									
ATOM 7133 CB GLN 3309 58,6225 -7.962 48,249 1.00 42,024 ATOM 7135 CC GLN 3309 59,594 -10.024 48,969 1.00 45,74 ATOM 7137 CD GLN 3309 59,594 -10.024 48,969 1.00 47,62 ATOM 7137 OEI GLN 3309 59,662 -11.135 50.011 1.00 49,24 ATOM 7137 OEI GLN 3309 59,662 -11.135 50.011 1.00 49,24 ATOM 7139 C GLN 3309 59,376 -12.865 49.587 1.00 42,99 ATOM 7140 O GLN 3309 55,058 -8.875 47.369 1.00 42,99 ATOM 7141 N LEE 3310 55,058 -8.749 46.055 1.00 41.35 ATOM 7141 CB LLE 3310 55,599 -9.338 45.097 1.00 42.99 ATOM 7142 CB LLE 3310 55,599 -9.338 45.097 1.00 40.29 ATOM 7144 CG2 LLE 3310 55,599 -9.338 45.097 1.00 41.04 ATOM 7145 CG1 LLE 3310 55,059 -9.166 43.550 1.00 41.04 ATOM 7146 CD1 LLE 3310 55,600 -6.672 43.306 1.00 41.77 ATOM 7146 CD1 LLE 3310 55,6498 -10.828 45.401 1.00 39.96 ATOM 7147 C LLE 3310 55,498 -10.828 45.401 1.00 39.96 ATOM 7148 O LLE 3310 55,498 -11.561 45.312 1.00 40.25 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.96 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.96 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 46.108 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 47.89 61.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 42.268 1.00 39.95 ATOM 7150 CA LEU 3311 55,095 -12.667 42.268 1.00 39.95 ATOM 7150 CA LEU 3311 50.00 39.95 ATOM 7150		MOTA	7132	N	GLN	3309	_					
ATOM 7134 CB GLN 3309 58,601 -8,932 49,366 1.00 47,62 ATOM 7135 CG GLN 3309 59,5694 -10.024 48,969 1.00 47,62 ATOM 7137 CB GLN 3309 59,9662 -11.135 50.011 1.00 49,10 1.00 ATOM 7137 CB GLN 3309 59,963 -10.888 51.844 1.00 50.26 ATOM 7138 NE2 GLN 3309 59,963 -10.888 51.844 1.00 50.26 ATOM 7140 C GLN 3309 57,179 -8,580 47,769 1.00 49,10 ATOM 7141 N LE 3310 57,528 -8,749 46,055 1.00 41,03 ATOM 7143 CB LLE 3310 55,528 -8,749 46,055 1.00 40,25 ATOM 7143 CB LLE 3310 55,528 -9,424 42,696 1.00 41,19 ATOM 7145 CG1 LLE 3310 55,925 9,424 42,696 1.00 41,19 ATOM 7147 C LLE 3310 55,639 -9,138 43,301 1.00 41,19 ATOM 7147 C LLE 3310 55,600 -6,676 43,306 1.00 41,19 ATOM 7147 C LLE 3310 55,405 -9,424 42,696 1.00 40,25 ATOM 7148 CB LEU 3311 55,095 -10,828 45,401 1.00 39,96 ATOM 7148 CB LEU 3311 55,095 -12,667 61,088 1.00 39,53 ATOM 7151 CB LEU 3311 55,095 -12,667 61,088 1.00 39,53 ATOM 7151 CB LEU 3311 55,095 -12,667 61,088 1.00 39,53 ATOM 7153 CD1 LEU 3311 53,406 -12,251 49,630 1.00 39,14 ATOM 7155 CD LEU 3311 53,406 -12,251 49,630 1.00 39,14 ATOM 7156 CD LEU 3311 54,519 -13,484 49,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,519 -13,484 49,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,519 -13,484 49,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,519 -13,484 49,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,619 -13,484 49,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,619 -13,484 44,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,619 -13,484 44,974 1.00 39,14 ATOM 7156 CD LEU 3311 54,619 -13,484 44,974 1.00 39,14 ATOM 7156 CD LEU			7133	CA	GLN	3309						
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ATOM 7176 C ALA 3314 51.558 -12.590 35.417 1.00 36.40 ATOM 7177 O ALA 3314 52.370 -11.674 35.280 1.00 36.33 ATOM 7178 N GLY 3315 51.410 -13.562 34.528 1.00 35.90 55 ATOM 7179 CA GLY 3315 52.199 -13.596 33.311 1.00 36.63 ATOM 7180 C GLY 3315 51.986 -14.947 32.667 1.00 37.06 ATOM 7181 O GLY 3315 51.132 -15.716 33.119 1.00 37.82 ATOM 7182 N VAL 3316 52.745 -15.262 31.627 1.00 37.82 ATOM 7183 CA VAL 3316 52.745 -15.262 31.627 1.00 37.55 ATOM 7184 CB VAL 3316 52.560 -16.560 30.975 1.00 38.82 ATOM 7185 CG1 VAL 3316 53.239 -18.125 29.142 1.00 38.87	20							50.662 -1	2.676		1.00	37.04
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ATOM 7185 CG1 VAL 3316 53.239 -18.125 29.142 1.00 38.87	60					3316	•					
				CG1								
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٠ .	ATOM	7376	C	THR		•	48.403	-4.098 -6.912		
5	ATOM ATOM	7377 7378		THR	_		49.047	-7.583	47.232	1.00 31.96
	ATOM	7379		CYS CYS			46.965 46.597	-6.729 -7.248	– • •	
	ATOM	7380	CB				45.227	-7.900		
10	ATOM	7381			3341		44.857	-8.553	44.389	
10	ATOM ATOM	· 7382 7383		CYS			46.558	-6.037	45.035	1.00 32.96
	ATOM	7384	N	CYS LEU	3341 3342		45.682 47.513	~5.183 ~5.971	45.158	
	ATOM	7385	CA	LEU			47.616	-4.858	44.116 43.189	1.00 32.48 1.00 32.48
15	MOTA	7386	СВ	LEU	3342		49.076	-4.407	43.135	1.00 32.46
13	ATOM ATOM	7387 7388	CG CD	LEU	3342		49.454	-3.104	42.430	1.00 34.51
	ATOM	7389	CD		3342 3342		49.092 50.952	-1.912 -3.099	43.303	1.00 34.35
	MOTA	7390	C	LEU	3342		47.134	-5.263	42.176 41.791	1.00 35.12 1.00 32.09
20	MOTA	7391	0	LEU	3342		47.558	-6.283	41.253	1.00 32.09
20	ATOM ATOM	7392 7393	N	ALA	3343		46.250	-4.469	41.200	1.00 31.02
v	ATOM	7394	CA CB	ALA ALA	3343 3343		45.739 44.328	-4.784	39.868	1.00 30.21
,}	MOTA	7395	c	ALA	3343		45.717	-5.375 -3.541	39.966 38.997	1.00 29.15 1.00 30.06
26	ATOM	7396	0	ALA	3343		45.231	-2.489	39.409	1.00 30.00
25	ATOM ATOM	7397	N	GLY	3344		46.242	-3.648	37.786	1.00 29.35
•	ATOM	7398 7399	CA C	GLY GLY	3344 3344		46.219	-2.491	36.918	1.00 29.15
	ATOM	7400	ŏ	GLY	3344		46.026 46.191	-2.823 -3.971	35.456 35.033	1.00 29.17. 1.00 29.56
20	MOTA	7401	N	ASN	3345		45.631	-1.813	34.690	1.00 29.38
30	MOTA MOTA	7402	CA	ASN	3345		45.459	-1.944	33.250	1.00 28.57
	ATOM	7403 7404	CB CG	asn Asn	3345 3345		44.006	-2.248	32.859	1.00 28.07
	ATOM	7405	OD1		3345		43.018 43.270	-1.228 -0.018	33.377 33.356	1.00 29.42 1.00 29.45
25	ATOM	7406		ASN	3345		41.863	-1.712	33.827	1.00 29.45
35	ATOM ATOM	7407	C	ASN	3345		45.933	-0.615	32.672	1.00 29.54
	ATOM	7408 7409	O N	ASN SER	334 ⁻ 5 3346		46.382 45.851	0.257	33.420	1.00 29.62
	ATOM	7410	CA	SER	3346		46.340	-0.442 0.797	31.359 30.758	1.00 30.06 1.00 30.55
40	ATOM	7411	СВ	SER	3346		46.133	0.781	29.235	1.00 30.53
40	ATOM ATOM	7412 7413	OG	SER	3346		45.062	1.619	28.836	1.00 31.68
	ATOM	7413	0	SER SER	3346 3346		45.714 46.365	2.047 3.087	31.364	1.00 31.09
	MOTA	7415	N.	ILE	3347		44.466	1.944	31.450 31.811	1.00 32.05 1.00 31.38
. 45	ATOM	7416	CA	ILE	3347		43.765	3.089	32.399	1.00 31.08
45	ATOM ATOM	7417 7418	CB	ILE	3347	:	42.232	2.891	32.326	1.00 30.92
•	ATOM	7419	CG2 CG1	ILE	3347 3347		41.524 41.816	4.096	32.941	1.00 29.41
	ATOM	7420		ILE	3347			2.688 2.016	30.862 30.663	1.00 29.84 1.00 29.21
50	ATOM.	7421	С	ILE	3347		44.136	3.454	33.839	1.00 31.37
50 ·	ATOM	7422	0	ILE	3347		44.069	4.630	34.206	1.00 31.86
	ATOM ATOM	7423 7424	n Ca	GLY GLY	3348 3348		44.518	2.474	34.656	1.00 31.56
	ATOM	7425	C	GLY	3348		44.874 45.158	2.785 1.612	36.034 36.964	1.00 31.39
~ ~	ATOM	7426	0	GLY	3348		45.062	0.440	36.570	1.00 32.13 1.00 32.10
55	ATOM	7427	N	LEU	3349		45.510	1.933	38.211	1.00 32.34
	ATOM ATOM	7428 7429	CA CB	LEU	3349		45.815	0.924	39.228	1.00 32.22
	ATOM	7430	CG	LEU LEU	3349 3349		47.237 48.377	1.091 0.584	39.766	1.00 32.93
	MOTA	7431	CD1		3349		48.439	1.372	38.891 37.595	1.00 34.83 1.00 35.45
60	ATOM	7432	CD2		3349		49.679	0.730	39.650	1.00 35.43
	ATOM ATOM	7433	C	LEU	3349 .		44.851	0.911	40.412	1.00 31.88
•	TT ON	7434	0	LEU	3349		44.263	1.925	40.783	1.00 31.99

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ATOM
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                                SER
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5	ATOM	8245	CB	HIS	4241	46.825 -11.496	83.705	1.00 41.26
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	ATOM	8251 8252		HIS	4241	47.895 -11.994	81.528	1.00 40.25
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15	ATOM	8255		THR	4242	47.631 -13.431	79.266 78.433	1.00 37.65 1.00 37.75
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	ATOM	8257	CG2		4242	47.729 -13.023	76.969	1.00 37.80
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	ATOM	8263		TYR	4243	44.004 -8.612	79.216	1.00 33.78
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25	MOTA	8265	CE1		4243	44.761 -7.524	81.244	1.00 33.55
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	ATOM ATOM	8267 8268		TYR	4243	42.635 -8.634	81.212	1.00 33.61
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	MOTA	8276	CD (GLN	4244	42.248 -13.502	71.181	1.00 42.27
	ATOM	8277	OE1		4244	41.644 -14.305	71.908	1.00 44.10
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40	ATOM	8279		GLN	4244	42.789 -9.631	73.231	1.00 33.75
40	ATOM	8280		GLN	4244	41.683 -9.278	73.638	1.00 33.38
	ATOM ATOM	8281 8282		LEU	4245	43.471 -8.968	72.309	1.00 32.82
	ATOM	8283		LEU LEU	4245 4245	42.932 -7.780 43.960 -6.650	71.681	1.00 32.23
	ATOM	8284		LEU	4245	43.625 -5.419	71.709 70.849	1.00 32.31 1.00 33.45
45	ATOM	8285		LEU	4245	42.283 -4.840	71.259	1.00 33.45
	ATOM	8286		LEU	4245	44.734 -4.371	70.990	1.00 32.44
	ATOM	8287		LEU	4245	42.540 -8.075	70.246	1.00 31.65
	ATOM	8288	0 1	LEU	4245	43.340 -8.569	69.452	1.00 31.23
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50	ATOM	8290	CA A	ASP	4246	40.782 -7.983	68.579	1.00 31.60
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	MOTA	8292		ASP	4246	39.308 -9.500	67.210	1.00 31.57
	ATOM	8293	OD1 /		4246	38.394 -10.347	67.114	1.00 31.79
55	ATOM	8294	OD2 I		4246	39.899 -9.005	66.221	1.00 29.97
J J	ATOM .	8295		ASP	4246	40.195 -6.665	68.075	1.00 31.32
	ATOM ATOM	8296 8297		ASP VAL	4246 4247	39.348 -6.066	68.737	1.00 31.34
	ATOM	8298		VAL VAL	4247	40.667 -6.203 40.178 -4.957	66.921	1.00 30.94
	ATOM	8299		VAL	4247	40.178 -4.957 41.336 -4.007	66.341 65.953	1.00 30.64
60	ATOM	8300	CG1 V		4247	40.794 -2.759	65.302	1.00 29.76 1.00 28.69
	ATOM	8301	CG2, V		4247	42.135 -3.645	67.170	1.00 28.69
	ATOM	8302		/AL	4247	39.378 -5.282	65.084	1.00 23.88
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	ATOM	8304	N	VAL			38.156	-4.757	65.010	1.00 32.25
•	ATOM	8305					37.264	-4.989	63.867	1.00 32.28
	ATOM	8306		VAL			35.873	-5.501	64.340	
5	MOTA	8307			4248		34.888	-5.492	63.190	1.00 32.43
_	ATOM	8308	CG		4248		35.990	-6.896		1.00 32.46
	ATOM	8309		VAL	4248				64.891	1.00 33.47
	ATOM	8310					37.019	-3.693	63.081	1.00 33.17
				VAL	4248		36.651	-2.689	63.660	1.00 33.40
10	ATOM	8311	N	GLU	4249		37.182	-3.679	61.768	1.00 33.84
10	MOTA	8312	CA	GLU	4249		36.924	-2.425	61.045	1.00 34.40
	ATOM	8313	CB	GLŲ	4249		37.877	-2.309	59.847	1.00 34.83
	ATOM	8314	CG	GLU	4249		39.344	-2.426	60.256	1.00 36.55
	ATOM	8315	CD	GLU	4249		40.318	-2.056	59.150	1.00 39.13
	ATOM	8316	OE:	L GLU	4249		40.634	-2.920	58.297	1.00 40.64
15	ATOM	8317	OE2	GLU	4249		40.771	-0.888	59.130	1.00 39.71
	ATOM	8318	С	GLU	4249		35.458	-2.320	60.596	1.00 33.65
	ATOM	8319	0	GLU	4249		34.837	-3.333	60.278	
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20	ATOM	8322	CB	ARG	4250		33.504	-0.914	60.182	1.00 33.16
20	ATOM	8323					32.709	-0.118	61.232	1.00 32.28
			CG	ARG	4250	-	32.700	-0.684	62.657	1.00 31.28
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	ATOM	8325	NE	ARG	4250		31.024	-2.499	62:245	1.00 30.24
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25	ATOM	8327		ARG	4250		29.965	-1.883	64.196	1.00 31.16
	ATOM	8328	NH2	ARG	4250		28.743	-2.718	62.451	1.00 31.07
•	MOTA	· 8329	С	ARG	4250		33.414	-0.178	58.834	1.00 34.09
	ATOM	8330	0	ARG	4250		34.352	0.514	58.434	1.00 34.30
	ATOM	8331	N	SER	4251		32.287	-0.341	58.141	1.00 34.95
30	ATOM	8332	CA	SER	4251		32.043	0.304	56.846	1.00 35.73
	ATOM	8333	CB	SER	4251		32.136	-0.706	55.709	1.00 35.73
	ATOM	8334	OG	SER	4251		33.432		55.655	1.00 38.10
	ATOM	8335	Ċ	SER	4251		30.653	0.918	56.827	1.00 35.10
	MOTA	8336	Ö	SER	4251		29:698	0.288		
35	ATOM	8337	N	PRO	4252		30.529		56.389	1.00 36.05
	ATOM	8338	CD	PRO	4252			2.165	57.298	1.00 36.23
	ATOM	8339	CA	PRO	4252		31.640	2.988	57.810	1.00 35.96
	ATOM	8340					29.266	2.907	57.358	1.00 36.03
	ATOM		CB	PRO			29.559	3.964	58.411	1.00 35.84
40		8341	· CG	PRO	4252		30.962	4.337	58.067	1.00 36.40
TU	MOTA	8342	C	PRO	4252		28.885	3.520	56.011	1.00 36.05
	MOTA	8343	0	PRO	4252		28.773	4.739	55.877	1.00 36.52
	ATOM	8344	N	HIS	4253		28.691	2.665	55.016	1.00 35.94
	MOTA	8345	CA	HIS	4253		28.328	3.093	53.666	1.00 35.62
45	ATOM	8346	CB	HIS	4253		29.478	2.884	52.679	1.00 38.03
45	ATOM	8347	CG	HIS	4253		30.715	3.657	52.996	1.00 42.01
	ATOM	8348		HIS	4253		31.282	4.720	52.377	1.00 43.13
	ATOM	8349	ND1	HIS	4253		31.542	3.340	54.054	1.00 44.01
	ATOM	8350	CE1	HIS	4253		32.567	4.176	54.071	1.00 44.30
	ATOM	8351	NE2	HIS	4253		32.434	5.022	53.064	1.00 44.43
50	ATOM	8352	С	HIS	4253		27.195	2.233	53.154	1.00 34.14
	ATOM	8353	Ō	HIS	4253		26.943	1.150	53.674	1.00 33.82
	ATOM	8354	N	ARG	4254		26.539	2.702		
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55	ATOM	8357	CG	ARG	4254		24.775	2.743	50.410	1.00 31.74
55	ATOM						25.624	3.051	49.205	1.00 31.47
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                                          12.492
                                                   -3.973
                                                            42.145
                                                                     1.00 38.20
                                                                     1.00 36.16
1.00 35.34
1.00 37.15.
   · ATOM
              8641
                                                   ~7.283 .
                    С
                         LEU
                               4290
                                          13.523
                                                            38.539
30
     ATOM
              8642
                                                            38.008
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                         LEU
                               4290.
                                          14.636
                                                   -7.363
   · ATOM
              8643
                         LYS
                                                   -7.376
                    N
                               4291.
                                          12.379
                                                            37.872
      ATOM
              8644
                    CA
                         LYS
                               4291
                                          12.323
                                                   -7.514
                                                            36.423
                                                                     1.00 38.48
     ATOM
              8645
                    CB
                         LYS
                              4291
                                          11.609
                                                   -8.817
                                                            35.026
                                                                     1.00 39.76
                                         11.108
              8646
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      ATOM
                    ÇG
                         LYS
                               4291
                                                   -8.901
                                                                     1.00 40.60
35
              8647
                    CD
      MOTA
                         LYS
                              4291
                                          12.246
                                                   -8.830
                                                            33.535
                                                                     1.00 42.97
              8648
      MOTA
                    CE
                        LYS
                              4291
                                          11.820
                                                   -9.328
                                                            32.138
                                                                     1.00 44.27
                                          10.669
11.541
      MOTA
              8649
                         LYS
                              4291
                                                   ~8.590
                    NZ
                                                            31.524
                                                                     1.00 44,72
      ATOM
              8650
                    С
                         TA3
                              4291
                                                   -6.306
                                                            35.924
                                                                     1.00 38.86
                                                            36.390
35.007
      ATOM
              8651
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                         LYS
                              4291
                                          10.430
                                                   ~6.043
                                                                     1.00 37.83
40
              8652
                                          12.142
      ATOM
                    N
                         HIS
                              4292
                                                   -5.556
                                                                     1.00 40.21
      MOTA
              8653
                    CA
                              4292
                        HIS
                                          11.490
                                                   -4.384
                                                                     1.00 42.41
                                                            34.433
      MOTA
              8654
                              4292
                                          12.525
                    CB
                        HIS
                                                   -3.516
                                                            33.725
                                                                     1.00 41.96
              8655
                                                                     1.00 41.96
1.00 42.64
      MOTA
                    CG
                         HIS
                              4292
                                          13.440
                                                   -2.809
                                                            34.668
                    CD2 HIS
      MOTA
              8656
                              4292
                                          14.624
                                                   -3.182
                                                            35.207
45
              8657
                              4292
     ATOM
                    ND1 HIS
                                          13.104
                                                  -1.617
                                                            35.267
36.141
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             8658
     ATOM
                    CE1 HIS
                              4292
                                          14.038
                                                   -1.288
                                                                     1.00 42.75
                                                  -2.221
     MOTA
              3659
                    NE2 HIS
                              4292
                                          14.971
                                                            36,126
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     MOTA
             8660
                    С
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                              4292
                                                            33.471
                                          10.395
                                                   -4.826
                                                                     1.00 44.25
                                                            32.507
33.761
     MOTA
             8661
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                                          10.652
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     ATOM
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                                           9.180
                                                  -4.366
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     ATOM
             8663
                    ÇA
                        ILE
                              4293
                                           7.979
                                                  -4.708
                                                                     1.00 51.04
     ATOM
             8664
                    СВ
                        ILE
                              4293
                                           6.918
                                                  -5.343
                                                            33.965
                                                                     1.00 51.20
                    CG2 ILE
                                                  -5.771
-6.568
                                                                     1.00 51.79
     MOTA
             8665
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                                           5.679
                                                            33.198
                              4293
             8666
                                           7.509
     ATOM
                    CG1 ILE.
                                                            34.652
                                                                     1.00 51.93
55
     ATOM
             8667
                    CD1 ILE
                              4293
                                           8.030
                                                  -7.621
                                                            33.680
                                                                     1.00 52.28
     ATOM
             8668
                    С
                        ILE
                              4293
                                                  -3.524
                                           7.321
                                                            32.296
                                                                     1.00 53.15
                                                  -2.354
     MOTA
             8669
                    0
                        ILE
                              4293
                                           7.620
                                                            32.574
                                                                     1.00 53.09
     ATOM
             8670
                         GLU
                              4294
                                                            31.376
                                                                     1.00 55.65
                                           6.416
                                                  -3.857
     MOTA
             8671
                    CA
                        GLU
                                                  -2.870
                              4294
                                           5.657
                                                            30.618
                                                                     1.00 58.14
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     ATOM
             8672
                    CB
                        GLU
                              4294
                                           5.801
                                                  -3.117
                                                            29.112
                                                                    1.00 57.19
     ATOM
             8673
                        GLU
                              4294
                    C
                                                  -2.960
                                           4.183
                                                            31.012
                                                                     1.00 59.77
     MOTA
             8674
                        GLU
                              4294
                                           3.759
                                                  -3.897
                                                            31.689 1.00 59.44
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	MOTA	8675	N	VAL	4295		3.413	-1.967	30.593		62.69
	MOTA	8676	CA	VAL	4295		1.981	-1.915	30.868		65.41
5	MOTA	8677	CB	VAL	4295		1.700	-1.091	32.152	1.00	65.44
	MOTA	8678	CG1		4295		0.211	-0.817	32.307		65.73
	MOTA	8679		VAL	4295		2.211	-1.861	33.366		64.96
	MOTA	8680	C	VAL	4295		1.323	-1.287	29.636		67.29
	MOTA	8681	0	VAL	4295		0.118	-1.025	29.611		67.51
•	ATOM	8682	N	ASN	4296		2.154	-1.083	28.612		69.59
10	ATOM	8683	CA	ASN	4296		1.786	-0.515	27.311	1.00	
10	MOTA	8684	CB	ASN	4296		1.279	0.925	27.459		72.56
	MOTA	8685	CG	ASN	4296		-0.044	1.004	28.180	1.00	73.76
	MOTA	8686		ASN	4296		-1.025	0.378	27.767	1.00	
•	ATOM	8687		ASN	4296		-0.082	1.766	29.273	1.00	74.09
15	ATOM ATOM	8688	C	ASN	4296		3.067	-0.498	26.482	1.00	
13	ATOM	8689	0	ASN	4296		3.666	-1.540	26.200	1.00	73.05
	ATOM	8690 8691	N CA	GLY	4297		3.467	0.705	26.089		73.53
20	ATOM	8692		GLY	4297		4.698	.0.898	25.349	1.00	74.28
	ATOM	8693	C	GLY	4297		5.497	1.723	26.338		74.92
	ATOM	8694	N O		4297		6.571	2.267	26.039	1.00	74.91
	ATOM	8695	CA	SER SER	4298		4.924	1.806	27.540		74.92
	ATOM	8696	CB	SER.	4298 4298		5.496	2.548	28.652		74.63
25	ATOM	8697	OG	SER	4298			3:393	29.335		74.57
	ATOM	8698	. C	SER	4298		3.226 6.164	2.642	29.564		75.04
	ATOM	8699	Ö	SER	4298		5:498	1.624 0.876	29.667		74.22
	ATOM	8700	N	LYS	4299		7.493	1.676	30.388	1.00	
	ATOM	8701	CA	LYS	4299		8.285	0.884	29.689 30.611		73.81
	ATOM	8702	CB	LYS	4299		9.704	0.700	30.070		73.37 73.41
	ATOM	8703	CG	LYS	4299		9.779	-0.112	28.783		73.41
30	ATOM	8704	CD	I,YS	4299		11.219	-0.283	28.314		73.93
	ATOM	8705	CE	LYS	4299		11.301	-1.171	27.074		74.43
	ATOM	8706	NZ	LYS	1299		12.705	-1.372	26.596		74.54
	ATOM	8707	С	LYS	4299		8.318	1.655	31.920		72.94
•	ATOM	8708	0	LYS	4299		8.678	1.119	32.969		73.16
35	ATOM	8709	N	ILE	4300		7.932	2.924	31.841		72.42
	ATOM	8710	CA	ILE	4300		7.893	3.798	33.003		72.36
	ATOM	8711	CB	ILE	4300		8.580	5.153	32.717		72.06
40	ATOM	8712	CG2	ILE	4300		8.693	5.967	34.002		71.81
	ATOM	8713		ILE	4300		9.974	4.920	32.136		71.69
	ATOM	8714	CD1	ILE	4300		10.901	4.157	33.055		72.04
	ATOM	8715	C	ILE	4300		6.434	4.050	33.359		72.49
	ATOM '	0,20	0	ILE	4300		5.548	3.904	32.517	1.00	72.30
45	MOTA	8717	N	GLY	4301		6.193	4.424	34.609		72.80
	ATOM	8718	CA	GLY	4301.		4.838	4.680	35.057	1.00	73.35
43	ATOM	8719	C	GLY	4301		4.440	6.147	35.057	1.00	73.57
	ATOM	8720	0	GLY	4301		5.252	7.022	34.731		73.30
	ATOM	8721	N	PRO	4302		3.179	6.444	35.426		73.73
	ATOM ·	8722	CD	PRO	4302		2.148	5.443	35.742	1.00	73.72
50	ATOM	8723	CA	PRO	4302		2.613	7.801	35.485	1.00	
30	ATOM	8724	CB	PRO	4302		1.111	7.550	35.656	1.00	73.95
	MOTA MOTA	8725	CG	PRO	4302		0.918	6.109	35.202	1.00	
	ATOM	8726 8727	C	PRO	4302		3.189	8.579	36.659		72.79
	ATOM	8728	0	PRO	4302		2.988	9.791	36.781		72.49
55	ATOM	8729	N CA	ASP ASP	4303		3.901	7.856	37.520		72.01
J J	ATOM	8729 8730	CA		4303 4303		4.529	8.429	38.701		71.14
	ATOM	8731	CB	ASP			4.234	7.553	39.925		71.50
60	ATOM	8732		ASP	4303		4.633	6.100	39.715		71.75
	ATOM	8733	OD1 OD2		4303		4.619	5.333	40.701		71.77
	ATOM	8734			4303		4.957	5.724	38.566		72.03
	ATOM	8735	C 0	ASP ASP	4303		6.043	8.566	38.510		70.24
	ATOM	8736	N	ASP	4303 4304	•	6.775	8.824	39.470		70.13
	014	0,30	74	LTO [A	4304		6.501	8.383	37.271	1.00	68.93

ATOM 8739 CB ASN 4304 8.505 9.789 37.552 1.00 67.87 ATOM 8730 CG ASN 4304 10.157 10.121 37.047 1.00 68.24 ATOM 8740 NDZ ASN 4304 10.157 10.142 35.835 1.00 67.87 ATOM 8741 NDZ ASN 4304 10.157 10.142 35.835 1.00 67.87 ATOM 8742 C ASN 4304 8.744 7.277 37.351 1.00 66.27 ATOM 8743 O ASN 4304 8.744 7.277 37.351 1.00 66.27 ATOM 8743 CA LEU 4305 8.106 6.352 38.059 1.00 64.57 ATOM 8745 CA LEU 4305 8.106 6.352 38.059 1.00 64.57 ATOM 8746 CB LEU 4305 8.261 4.681 39.859 1.00 62.93 ATOM 8746 CB LEU 4305 8.261 4.681 39.859 1.00 62.93 ATOM 8748 CDL LEU 4305 8.261 4.681 39.859 1.00 62.93 ATOM 8749 CDL LEU 4305 8.261 4.681 39.859 1.00 62.83 ATOM 8749 CDL LEU 4305 8.261 4.681 39.859 1.00 62.83 ATOM 8740 CDL LEU 4305 8.261 4.681 39.859 1.00 62.83 ATOM 8740 CDL LEU 4305 8.251 4.681 39.859 1.00 62.83 ATOM 8750 C LEU 4305 8.517 4.039 37.455 1.00 63.05 ATOM 8750 C LEU 4305 8.517 4.039 37.455 1.00 63.05 ATOM 8755 CD LEU 4305 8.517 4.039 37.455 1.00 63.05 ATOM 8755 CD PRO 4306 19.336 3.216 37.156 1.00 62.08 ATOM 8755 CD PRO 4306 19.933 3.366 37.688 1.00 62.08 ATOM 8755 CD PRO 4306 19.335 2.134 36.176 1.00 62.08 ATOM 8755 CD PRO 4306 19.395 2.134 36.176 1.00 62.08 ATOM 8755 CD PRO 4306 10.923 3.366 37.688 1.00 65.12 ATOM 8755 CD PRO 4306 10.592 3.366 37.688 1.00 65.12 ATOM 8755 CD PRO 4306 10.592 3.366 37.688 1.00 65.12 ATOM 8755 CD PRO 4306 10.592 3.366 37.688 1.00 65.12 ATOM 8755 CD PRO 4306 8.847 0.499 37.854 1.00 55.10 57.26 ATOM 8755 CD PRO 4306 8.847 0.499 37.854 1.00 55.10 57.26 ATOM 8755 CD PRO 4306 8.847 0.499 37.854 1.00 55.50 57.26 ATOM 8765 CD TYR 4307 6.986 -0.253 38.835 1.00 60.44 57.26 ATOM 8765 CD TYR 4307 6.986 -0.253 38.835 1.00 60.44 57.26 ATOM 8766 CB TYR 4307 6.986 -0.253 38.835 1.00 60.43 ATOM 8766 CB TYR 4307 7.257 0.324 35.885 1.00 55.34 ATOM 8766 CB TYR 4307 7.250 -2.214 35.375 1.00 55.34 ATOM 8766 CB TYR 4307 7.250 -2.214 35.375 1.00 55.34 ATOM 8766 CB TYR 4307 7.250 -2.217 33.863 1.00 60.43 ATOM 8766 CB TYR 4307 7.250 -2.251 33.863 1.00 60.43 ATOM 8779 CB LEU 4308 9.00 -2.207 33.863 1.00 60.43 ATOM 8779 CB LEU		ATOM	8737	CA	ASN	4304		7.92	4 8.503	36.928	1.00 67.67
ATCM 8740 001 ASN 4304 9,905 10.121 37,047 1.00 68.24 ATCM 8740 001 ASN 4304 10.820 10.403 37.979 1.00 67.71 ATCM 8742 C ASN 4304 10.820 10.403 37.979 1.00 67.71 ATCM 8743 O ASN 4304 9.934 7.177 37.044 1.00 66.27 ATCM 8743 N LEU 4305 8.106 6.352 38.059 1.00 64.57 ATCM 8745 CB LEU 4305 8.776 5.131 38.490 1.00 62.73 ATCM 8746 CB LEU 4305 8.766 6.352 38.059 1.00 62.73 ATCM 8746 CD LEU 4305 8.766 5.131 38.490 1.00 62.73 ATCM 8748 CD LEU 4305 8.766 5.131 38.490 1.00 62.73 ATCM 8748 CD LEU 4305 8.769 5.458 41.074 1.00 62.83 ATCM 8749 CD LEU 4305 8.769 5.458 41.074 1.00 62.83 ATCM 8749 CD LEU 4305 8.261 4.681 39.858 1.00 63.05 1.06 ATCM 8749 CD LEU 4305 8.261 4.681 39.458 1.00 63.05 ATCM 8755 C LEU 4305 8.215 6.870 41.071 1.00 63.05 ATCM 8755 C PRO 4306 10.923 3.306 37.648 1.00 59.81 ATCM 8755 CB PRO 4306 10.923 3.306 37.648 1.00 59.81 ATCM 8755 CB PRO 4306 10.923 3.306 37.648 1.00 59.81 ATCM 8755 CB PRO 4306 10.923 3.306 37.648 1.00 59.81 ATCM 8755 CB PRO 4306 10.842 1.805 35.832 1.00 59.65 ATCM 8756 CB PRO 4306 10.842 1.805 35.832 1.00 59.65 ATCM 8758 C PRO 4306 8.637 0.916 36.712 1.00 65.02 ATCM 8756 CB PRO 4306 10.842 1.805 35.832 1.00 59.95 ATCM 8758 C PRO 4306 8.637 0.916 36.712 1.00 57.92 ATCM 8758 C PRO 4306 8.637 0.916 36.712 1.00 57.92 ATCM 8758 C PRO 4306 8.637 0.916 36.712 1.00 57.92 ATCM 8758 C PRO 4306 8.637 0.916 36.712 1.00 57.92 ATCM 8758 C PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.712 1.00 57.93 ATCM 8759 O PRO 4306 8.637 0.916 36.93 ATCM 8759 O PRO 4306 8.637 0.916 3		•		CB	ASN	4304					
ATOM 8740 ND2 ASN 4304 10.157 10.142 35.835 1.00 67.87 ATOM 8741 ND2 ASN 4304 10.820 10.403 37.979 1.00 67.87 ATOM 8743 O ASN 4304 9.934 7.177 37.351 1.00 66.27 ATOM 8745 CA LEU 4305 8.106 6.352 38.059 1.00 64.57 ATOM 8745 CA LEU 4305 8.106 6.352 38.059 1.00 64.57 ATOM 8747 CG LEU 4305 8.261 4.681 39.858 1.00 62.93 ATOM 8748 CD1 LEU 4305 8.261 4.681 39.858 1.00 62.93 ATOM 8748 CD1 LEU 4305 8.261 4.681 39.858 1.00 62.83 ATOM 8749 CD2 LEU 4305 8.261 4.681 39.858 1.00 62.83 ATOM 8749 CD2 LEU 4305 8.261 4.681 39.858 1.00 62.83 ATOM 8749 CD2 LEU 4305 8.251 6.870 41.071 1.00 62.05 ATOM 8750 C LEU 4305 8.517 4.039 37.456 1.00 62.05 ATOM 8750 C LEU 4305 8.517 4.039 37.456 1.00 62.05 ATOM 8751 C LEU 4305 8.517 4.039 37.456 1.00 62.05 ATOM 8751 C LEU 4305 9.536 3.216 37.156 1.00 60.36 ATOM 8752 CD PRO 4306 10.923 3.306 37.648 1.00 59.81 ATOM 8751 CD PRO 4306 10.923 3.306 37.648 1.00 59.81 ATOM 8755 CD PRO 4306 10.923 3.306 37.648 1.00 59.81 ATOM 8755 CD PRO 4306 10.923 3.306 37.648 1.00 59.81 ATOM 8755 CD PRO 4306 10.842 1.805 35.832 1.00 59.57 ATOM 8750 CD PRO 4306 8.637 0.916 36.712 1.00 57.26 ATOM 8750 CD PRO 4306 8.637 0.916 36.712 1.00 57.26 ATOM 8750 CD PRO 4306 8.637 0.916 36.712 1.00 57.26 ATOM 8760 CA TYR 4307 7.577 0.354 35.884 1.00 56.52 ATOM 8761 CC TYR 4307 7.577 0.354 35.884 1.00 56.52 ATOM 8763 CC TYR 4307 4.952 -0.221 34.785 1.00 57.26 ATOM 8763 CD TYR 4307 4.952 -0.221 34.785 1.00 57.23 ATOM 8763 CD TYR 4307 4.952 -0.221 34.785 1.00 55.10 ATOM 8765 CD TYR 4307 7.577 0.354 35.884 1.00 56.52 ATOM 8767 CZ TYR 4307 4.952 -0.221 34.785 1.00 57.23 ATOM 8767 CZ TYR 4307 4.952 -0.221 34.785 1.00 57.23 ATOM 8767 CZ TYR 4307 4.952 -0.221 34.785 1.00 57.25 ATOM 8767 CZ TYR 4307 4.952 -0.221 34.795 1.00 57.25 ATOM 8768 CD TYR 4307 7.575 0.354 35.884 1.00 60.44 ATOM 8768 CD TYR 4307 7.562 -1.248 35.151 1.00 57.26 ATOM 8768 CD TYR 4307 7.956 -2.258 35.809 1.00 61.23 ATOM 8769 CD TYR 4307 7.956 -2.258 35.809 1.00 61.33 ATOM 8769 CD TYR 4307 7.966 -2.258 35.809 1.00 61.33 ATOM 8777 CD TYR 4307 7.966 -2.258 35.809 1.00 6				CG	asn	4304		9.90			
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ATOM										41.045	1.00 62.06
15										41.071	1.00 63.05
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ATOM 8753 CD PRO 4306 9.395 2.134 36.176 1.00 59.81 ATOM 8755 CB PRO 4306 10.842 1.805 35.832 1.00 59.65 ATOM 8756 CG PRO 4306 11.530 2.007 37.153 1.00 59.65 ATOM 8757 C PRO 4306 8.637 0.916 36.712 1.00 57.26 ATOM 8758 0 PRO 4306 8.637 0.916 36.712 1.00 57.26 ATOM 8758 N TYR 4307 7.757 0.354 35.864 1.00 55.26 ATOM 8750 C PRO 4306 8.847 0.499 37.854 1.00 55.26 ATOM 8760 CA TYR 4307 7.757 0.354 35.984 1.00 55.25 ATOM 8761 CB TYR 4307 6.986 -0.825 36.278 1.00 55.51 ATOM 8762 CD TYR 4307 6.996 -0.825 36.278 1.00 57.23 ATOM 8763 CD TYR 4307 4.952 -0.221 34.785 1.00 57.23 ATOM 8763 CD TYR 4307 4.952 -0.221 34.785 1.00 59.93 ATOM 8763 CD TYR 4307 3.918 1.210 33.099 1.00 61.23 ATOM 8765 CD2 TYR 4307 3.918 1.210 33.099 1.00 61.23 ATOM 8765 CD2 TYR 4307 3.998 0.230 35.704 1.00 60.43 ATOM 8766 CE2 TYR 4307 3.998 0.230 35.704 1.00 60.43 ATOM 8766 CB TYR 4307 3.998 0.230 35.704 1.00 61.18 ATOM 8767 CZ TYR 4307 3.099 1.203 35.004 1.00 61.18 ATOM 8767 CZ TYR 4307 2.978 1.641 34.023 1.00 61.18 ATOM 8768 OH TYR 4307 2.978 1.641 34.023 1.00 61.18 ATOM 8768 OH TYR 4307 2.978 1.641 34.023 1.00 61.91 ATOM 8768 OH TYR 4307 2.905 2.536 33.630 1.00 61.91 ATOM 8767 CZ TYR 4307 7.962 -1.974 36.521 1.00 52.62 ATOM 8771 N VAL 4308 7.995 -2.479 37.750 1.00 49.77 ATOM 8776 CG VAL 4308 8.880 -3.588 38.007 1.00 47.43 ATOM 8775 CG2 VAL 4308 8.880 -3.588 38.007 1.00 47.43 ATOM 8775 CG2 VAL 4308 8.880 -3.588 38.421 1.00 47.53 ATOM 8779 CG VAL 4308 8.112 -4.723 38.747 1.00 46.29 ATOM 8779 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.691 1.00 45.31 ATOM 8780 CG GLN 4309 8.666 -5.916 38.491 1.00 5	13									36.921	1.00 62.08
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ATOM								10.923	3.306	37.648	1.00 59.81
ATOM								9.395	2.134		1.00 59.10
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								11.949	-11.904		
		ATOM .	8798	CG 1	LEU	4311		11.451	-11.245		1.00 36.92

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45	ATOM ATOM ATOM ATOM	8965 8966 8967 8968	N P CA P CB P	HE HE HE	4333 4333 4333 4333		10.167 - 10.515 - 9.925 - 10.707 -	15.722 14.410 14.225	25.435 24.903 23.499 22.430	1.00 1.00 1.00	52.58 52.88 53.24 53.47 54.45
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JU _.	ATOM ATOM ATOM ATOM	8972 8973 8974 8975	C P	HE HE	4333 4333 4333 4333		12.851 - 12.199 - 10.023 - 10.498 -	16.295 13.345	21.417 20.470 25.864 25.854	1.00 1.00 1.00 1.00	55.41 53.23
55	ATOM ATOM ATOM	8976 8977 8978	N G	LU LU	4334 4334 4334		9.082 -1 8.505 -1 7.313 -1	13.741 12.858	26.714 27.718 28.405	1.00 1.00 1.00	53.25 53.69
	ATOM ATOM ATOM	8979 8980 8981	CG G	LU LU	4334 4334 4334		6.222 -1 6.632 -1 7.535 -1	l4.105 l5.385	27.473 26.728 25.865	1.00 1.00 1.00	58.21 59.31
60	ATOM ATOM ATOM	8982 8983 8984	C G	LÜ	4334 4334 4334		6.041 -1 9.569 -1 9.624 -1	16.457 12.549	27.003 28.774 29.326	1.00 1.00 1.00	59.89 52.54

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10	ATOM	9862	CA	TYR	5236		28.529	27.151	102.271		56.71
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1.5	ATOM	9866	CE1		5236		28.580	24.315	105.829		62.15
15	ATOM	9867	CD2		5236		28.491		105.520	1.00	61.21
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	ATOM	9870	ОН	TYR	5236		27.378		107.883		63.37
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20	ATOM	9872	0	TYR	5236		29.779	28.830	101,135		56.53
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25	ATOM	9876	0	GLY	5237		29.319	25.707	97.553		53.09
25	MOTA	9877	N	SER	5238		29.739	27.538	96.301		51.67
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30	MOTA	9881	Ç	SER	5238		30.869	27.347	94.116	1.00	48.81
30	ATOM ·	9882	0	SER	5238		31.006	28.556	93.944	1.00	
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35	MOTA · MOTA	9885 9887	CG2	ILE	5239		34.340	27.142	94.440		45.08 .
JJ			CG1	ILE	5239		34.042	24.865	93.497		44.82
	MOTA MOTA	9888 9889		ILE ILE	5239 5239		35.295	24.380	94.191		44.96
•	ATOM	9890	Õ	ILE	5239		32.420 31.582	26.039	91.284		44.96
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40	MOTA	9892	CA	ASN	5240		32.937	25.778	90.227	1.00	44.15
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••	ATOM	9898	ō	ASN	5240		34.902	26.935	88.205	1.00	43.00
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_	ATOM	10042	С	LEU	5257		36.945			1.00	27.08
5	MOTA	10043	_	LEU	5257		36.280		42.272	1.00	26.56
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	ATOM	10045 10046		GLN GLN	5258 5258		34.992 34.720				29.50
•	ATOM	10047	CG	GLN	5258		33.244	19.772 20.209	42.453 42.628		30.10 32.78
10	ATOM	10048	CD	GLN	5258		33.089	21.748	42.862		34.25
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15	ATOM	10052	O N	GLN ALA	5258 5259		35.183 33.627	18.183	39.912	1.00	
	ATOM	10054	CA	ALA	5259		33.164	16.863 16.335	40.848		29.19
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	MOTA	10056	C	ALA	5259		32.831	17.482	38.619	1.00	
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	ATOM	10059	CA	GLY	5260		32.866	18.350	36.364	1.00	
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	ATOM	10062	N	GLY LEU	5260 5261		33.856 34.955	20.088	35.073		29.08
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30	ATOM ATOM	10068 10069	C	LEU	5261		37.388	19.816	36.637		29.09
	MOTA	10009	O N	LEU PRO	5261 5262		37.708	18.914	37.403		29.60
	ATOM	10071	CD	PRO	5262		38.227 39.586	20.273 19.733	35.693 35.492	1.00	29.52
	ATOM	10072	CA	PRO	5262		37.947	21.347	34.731	1.00	29.66 29.39
35 ··	MOTA	10073	CB	PRO	5262		39.324	21.659	34.155	1.00	
	ATOM	.10074	CG	PRO	5262		39.972	20.312	34.134		29.76
	MOTA	10075	Ç	PRO	5262		36.956	20.880	33.679	1.00	29.37
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	ATOM	10079	CB	ALA	5263		34.079	21.499 22.312	31.978 32.230	1.00	30.27 28.22
	ATOM	10080	C	ALA	5263		35.829	21.747	30.563	1.00	
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45	MOTA	10082	N	ASN	5264		35.309	20.979		1.00	32.00
43	ATOM ATOM	10083 10084	CA	ASN	5264		35.679	21.143	28.205	1.00	33.24
	ATOM	10085	CB CĠ	asn Asn	5264 5264		34.975 35.388	20.096	27.343	1.00	31.59
٠	ATOM	10086		ASN	5264		36.538	18.688 18.438	27.696	1.00	31.51
	ATOM	10087		ASN	5264		34.457	17.755	28.040 27.597	1.00	31.48 31.40
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	MOTA	10922	C2	SCR	2	34.282	-0.580	83.877	1.00 83.18
	ATOM	10923	C3	SCR	2	35.441	-1.532	83.558	1.00 82.73
	ATOM	10924	C4	SCR	2 ·.	35.593	-1.700	82.036	1.00 82.62
	ATOM	10925	C5	SCR	2	35.796	-0.317	81.390	1.00 82.27
20	MOTA	10926	C6	SCR	2	35.990	-0.134	79.895	1.00 81.13
	ATOM	10927	C11	SCR	2	35.298	3.226	85.281	1.00 88.41
	ATOM	10928	`C12	SCR	2	~35.723°	·· 2.863	83.845	1.00 87.56
	ATOM	10929		SCR	2	37.053	3.515	83.528	1.00 88.18
	ATOM	10930		SCR	2	37.006	3.704	82.040	1.00 87.83
25	MOTA	10931		SCR		35.587	4.136	81.792	1.00 87.50
	ATOM	10932		SCR	2	35.054	3.588	80.453	1.00 87.21
	ATOM	10933	01	SCR	2	35.7.04	1.426		
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		10934	02		2	34.138	-0.282	85.305	1.00 83.47
30	MOTA	10935		SCR	2	32.985	0.711	87.141	1.00 83.49
30	MOTA	10936	023	SCR	2	32.394	-1.518	86.459	1.00 83.42
	MOTA	10937		SCR	2	31.797	0.315	85.125	1.00 83.26
	MOTA	10938	03	SCR	2	35.243	-2.812	84.206	1.00 82.37
	ATOM	10339		SCR	2	35.864	-2.329	86.540	1.00 81.76
~ .	MOTA	10940	033	SCR	2	35.465	-4.562	85.796	1.00 81.88
35·	MOTA	10941	034	SCR	2	37.406	-3.328	85.118	1.00 81.45
	ATOM	10942	04	SCR	2	36.835	-2.427	81.935	1.00 83.31
	MOTA	10943	042	SCR	2	38.209	-4.145	81.220	1.00 83.75
	MOTA	10944	043	SCR	2	36.425	-3.485	79.920	1.00 84,12
•	MOTA	10945	044	SCR	2	36.068	-4.737	81.918	1.00 84.02
40	ATOM	10946	05	SCR	2	34.676	0.487	81.719	1.00 82.70
•	ATOM	10947	06	SCR	2	34.805	-0.334	79.134	1.00 79.99
	MOTA	10948	062		2	35.580	-1.352	77.104	1.00 79.12
	ATOM	10949	063	SCR	. 2	35.288	0.965	77.157	1.00 79.08
•	ATOM	10950	064	SCR	2	33.417	-0.404	77.280	1.00 79.43
45	ATOM	10951	010	SCR	2	34.839	3.526	82.889	
7.5	ATOM	10951		SCR	2				1.00 87.40
					2	33.907	4.333	79.927	1.00 87.19
	ATOM	10953		SCR	2	32.111	3.348	81.219	1.00 87.56
	ATOM	10954	053	SCR	2	32.401	2.839	78.895	1.00 86.88
50	ATOM	10955		SCR	2	31.623	4.913	79.571	1.00 87.09
50	ATOM	10956		SCR	2	38.044	4.600	81.599	1.00 87.77
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	MOTA	10958		SCR	2 2	38.075	3.769	79.331	1.00 88.02
	MOTA	10959	074	SCR	Ż	39.455	2.765	80.908	1.00 88.21
	ATOM	10960		SCR	2	34.705	4.561	85.371	1.00 90.35
55	ATOM	10961		SCR	2	33.481	4.335	87.389	1.00 91.50
	ATOM	10962	083		2	34.022	6.548	86.566	1.00 91.67
	ATOM	10963	084		2	35.699	5.174	87.434	1.00 91.07
	ATOM	10964	091		2	38.129	2.605	83.658	1.00 91.90
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5 0	MOTA		093		2	38.463	2.598	85.995	1.00 90.09
	MOTA	10967	094	SCR		39.585	4.197	84.556	1.00 90.29
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	END		0,	504	5005	24.541 -22.773	90.610	1.00 /9.18

WHAT IS CLAIMED IS:

1. An isolated composition comprising a ternary complex of:

- (a) an FGF ligand polypeptide;
- (b) an FGF receptor polypeptide; and
 - (c) a heparin agonist or antagonist,

wherein the heparin agonist or antagonist binds to the FGF ligand polypeptide and the FGF receptor polypeptide to form the ternary complex.

- 2. An isolated composition according to claim 1 in which the FGF ligand polypeptide is an FGF2 polypeptide having the amino acid sequence set forth in SEQ ID NO:1.
- 3. An isolated composition according to claim 1 in which the FGF receptor polypeptide is an FGFR1 polypeptide comprising residues 142-365 of the amino acid sequence set forth in SEQ ID NO:3.
- 4. An isolated composition according to claim 1 in which the heparin agonist or antagonist is a compound having the structure:

wherein R₁, R₂, R₃, R₄, R₅, R₆, R₇ and R₈ are independently benzyl, trityl, or - SO₃H.

5. An isolated composition according to claim 4 wherein at least one of R_1 , R_2 , R_3 , R_4 , R_5 , R_6 , R_7 and R_8 is a benzyl or trityl.

6. An isolated composition according to claim 4 in which the heparin agonist or antagonist is a heparin agonist.

- 7. An isolated composition according to claim 6 in which the heparin agonist is sucrose octasulfate (SOS).
- 8. An isolated composition according to claim 6 in which the heparin agonist is inositol hexasulfate or cyclodextrin.
- 9. An isolated composition according to claim 4 in which the heparin agonist or antagonist is a heparin antagonist.
- 10. An isolated composition according to claim 4 in which the heparin antagonist is a compound having the structure:

wherein R₄ and R₅ are independently benzyl, trityl, or SO₃H, and wherein at least one of R₄ and R₅ is benzyl or trityl.

- 11. An isolated composition according to claim 1 in which the ternary complex is dimerized.
- 12. An isolated composition according to claim 1 in which the ternary complex is dimer incompetent.
- 13. An isolated composition according to claim 1 in which molecules of the ternary complex have a crystalline structure.

14. An isolated composition according to claim 13 in which the crystalline structure has structure coordinates as set forth in the Appendix.

- 15. A method for identifying a compound that is an inhibitor of FGF receptor activity, which method comprises:
 - (a) designing a test compound, based on crystal structure coordinates for a ternary complex comprising (i) an FGF ligand polypeptide, (ii) an FGF receptor polypeptide, and (iii) a heparin agonist or antagonist that binds to the FGF ligand polypeptide and the FGF receptor polypeptide to form the ternary complex;
 - (b) synthesizing the designed test compound; and
 - (c) determining whether the test compound modulates FGF receptor activity.
 - 16. A method according to claim 15 in which:
 - (a) a first ternary complex and a second ternary complex are dimerized in the crystal structure coordinates; and
 - (b) the test compound is designed to form hydrogen bonds with the FGF receptor and ligand polypeptides in the first ternary complex, and also to form hydrogen bonds with an FGF receptor in the second ternary complex.
- 17. A method according to claim 15 in which the FGF receptor activity is a tyrosine kinase activity.
- 18. A method according to claim 15 in which the FGF receptor activity is an activity selected from the group consisting of mitogenesis and angiogenesis.
- 19. A method for inhibiting FGF receptor activity in a cell expressing an FGF receptor polypeptide, which method comprises contacting the cell with a compound in the presence of an FGF ligand so that FGF receptor activity in the cell is inhibited,

the compound having the structure:

wherein R_1 , R_2 , R_3 , R_4 , R_5 , R_6 , R_7 and R_8 are independently benzyl, trityl, or - SO_3H , and at least one of R_1 , R_2 , R_3 , R_4 , R_5 , R_6 , R_7 and R_8 is benzyl or trityl.

· · · · · · · 20.-- · · A method according to claim 19, wherein the compound has the structure · ·

wherein R_4 and R_5 are independently benzyl, trityl or -SO3H, and wherein at least one of R_4 and R_5 is benzyl or trityl.

- 21. A method according to claim 19 in which the FGF receptor activity is a tyrosine kinase activity.
- 22. A method according to claim 19 in which the FGF receptor activity is angiogenesis or mitogenesis.
- 23. A method for inhibiting dimerization of an FGF receptor polypeptide, which method comprises contacting the FGF receptor polypeptide to an admixture comprising (i) an FGF ligand, and (ii) having the structure:

wherein R₁, R₂, R₃, R₄, R₅, R₆, R₇ and R₈ are independently benzyl, trityl, or - SO₃H, and at least one of R₁, R₂, R₃, R₄, R₅, R₆, R₇ and R₈ is benzyl or trityl, so that dimerization of the FGF receptor polypeptide is inhibited.

24. A method according to claim 19, wherein the compound has the structure

wherein R_4 and R_5 are independently benzyl, trityl or -SO3H, and wherein at least one of R_4 and R_5 is benzyl or trityl.

- 25. A pharmaceutical composition comprising:
- (a) as compound having the structure:

$$R_2O$$
 R_4O
 OR_6
 OR_7
 OR_7
 OR_7
 OR_7
 OR_7

(b) a physiologically acceptable carrier or excipient,

wherein R_1 , R_2 , R_3 , R_4 , R_5 , R_6 , R_7 and R_8 are independently benzyl, trityl, or - SO_3H , and at least one of R_1 , R_2 , R_3 , R_4 , R_5 , R_6 , R_7 and R_8 is benzyl or trityl.

26. A pharmaceutical composition according to claim 25, wherein the compound has the structure:

wherein R_4 and R_5 are independently benzyl, trityl or -SO3H, and wherein at least one of R_4 and R_5 is benzyl or trityl.

27. An isolated composition according to claim 9, wherein the heparin antagonist is suramin.

1 maagsittlp alpedggsga fppghfkdpk rlycknggff lrihpdgrvd gvreksdphi 61 klqlqaeerg vvsikgvcan rylamkedgr llaskcvtde cffferlesn nyntyrsrky 121 tswyvalkrt gqyklgsktg pgqkailflp msaks

FIG. 1A

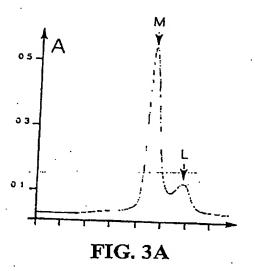
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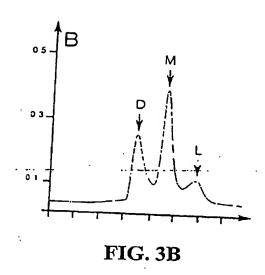
FIG. 1B

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301 gpdnlpyvqi lktagvnttd kemevlhlrn vsfedageyt clagnsigls hhsawltvle
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661 rlpvkwmape alfdriythq sdvwsfgvll weiftlggsp ypgvpveelf kllkeghrmd
721 kpsnctnely mmmrdcwhav psqrptfkql vedldrival tsnqeyldls mpldqyspsf
781 pdtrsstcss gedsvfshep lpeepclprh paqlangglk rr
```

FIG. 2A

```
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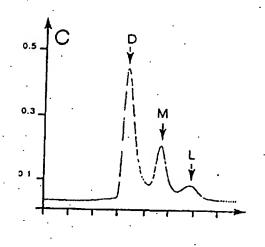


FIG. 3C

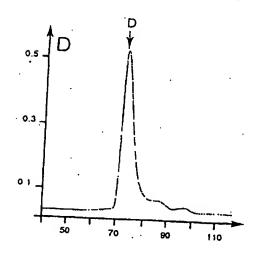


FIG. 3D

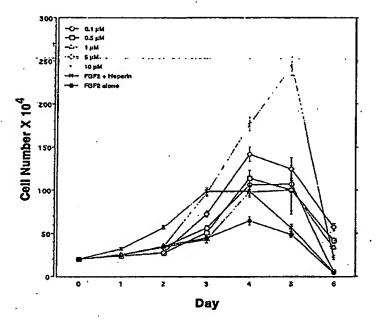


FIG. 4



FIG. 5A

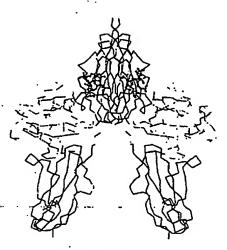


FIG. 5B





FIG. 5C

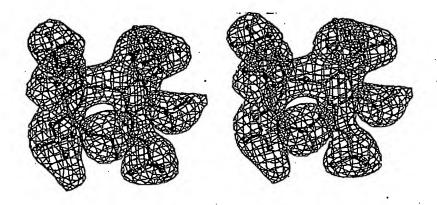


FIG. 6

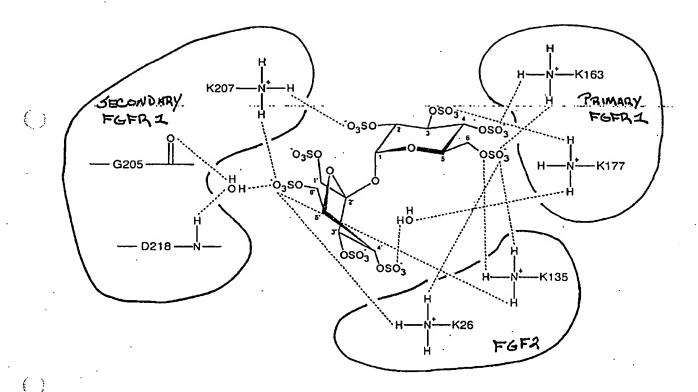


FIG. 7

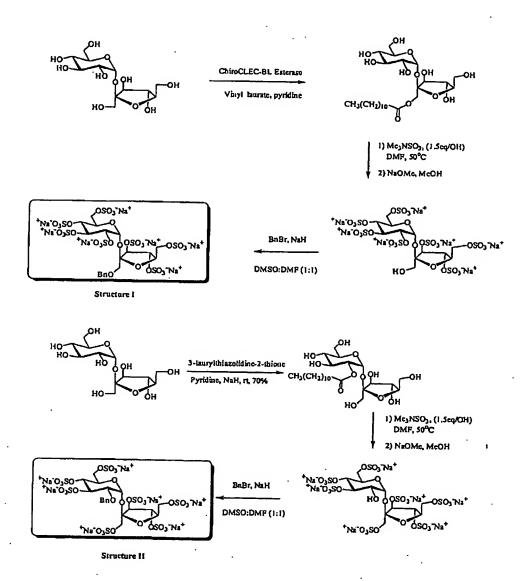


FIG. 8

Structre III

FIG. 9

FIG. 10

(_).

()

CH₃(CH₂)₁₀

•

CH₃(CH₂)₁₀

*Na*O3SO

(Structure VI)

FIG. 11

(CH₂)₁₄CH₃ Me₃NSO₃,(1.5eq/OH) DMF, 50°C

(Structure VII)

FIG. 12

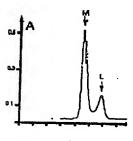


FIG. 13A

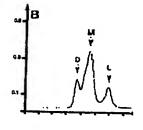


FIG. 13B

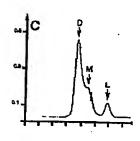


FIG. 13C

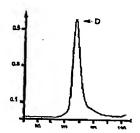


FIG. 13D.

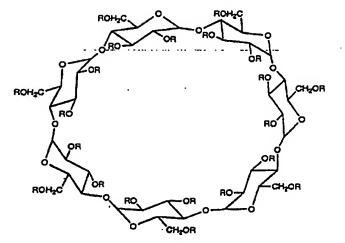


FIG. 14

FIG. 15A

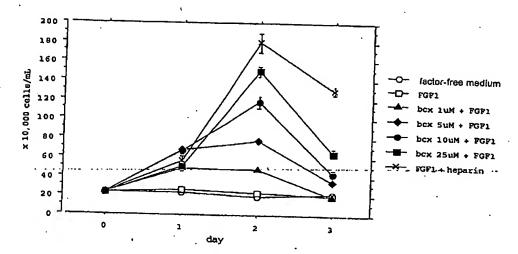


FIG. 15B

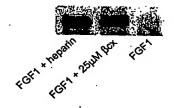


FIG. 15C



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FIG.16A

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FIG.16B

SEQUENCE LISTING

<110> New York University University of Iowa Moosa, Mohammadi Green, David L. Linhard, Robert J.

<120> STRUCTURE-BASED DESIGN AND SYSNTHESIS OF FGF INHIBITORS AND FGF MODULATOR COMPOUNDS

<130> 5986/2J277 WOO

<140> <141> To Be Assigned Herewith

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<170> PatentIn version 3.1

<210>

PRT

<213> Homo sapiens

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Val Asp Gly Val Arg Glu Lys Ser Asp Pro His Ile Lys Leu Gln Leu
50 60

Gln Ala Glu Glu Arg Gly Val Val Ser Ile Lys Gly Val Cys Ala Asn 65 75 80

Arg Tyr Leu Ala Met Lys Glu Asp Gly Arg Leu Leu Ala Ser Lys Cys 85 90 95

Val Thr Asp Glu Cys Phe Phe Phe Glu Arg Leu Glu Ser Asn Asn Tyr 100 105

Asn Thr Tyr Arg Ser Arg Lys Tyr Thr Ser Trp Tyr Val Ala Leu Lys 125

Arg Thr Gly Gln Tyr Lys Leu Gly Ser Lys Thr Gly Pro Gly Gln Lys 130 140

Ala Ile Leu Phe Leu Pro Met Ser Ala Lys Ser

60

120

180

240

300

360

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